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Machine Learning for Accelerating Development of Ion Conducting Membranes for Fuel Cell Applications

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ABSTRACT

Fuel cells such as polymer electrolyte membrane fuel cells are playing crucial role in the transition towards sustainable energy systems. Ion conducting membranes (ICMs) are playing critical chemical and mechanical roles in such fuel cells which directly affecting the efficiency, durability and overall device performance. Recent progress in machine learning (ML) is introducing powerful tools to aid in the discovery, design, and optimization of membrane materials that is likely to lead to quicker and more cost-effective materials development cycles. This article discusses the significant potential of applying ML research and development of new generation of ICMs for polymer electrolyte membrane fuel cells. The scope is overviewing types of polymer electrolyte membrane fuel cells and their operation environments with different ICMs in addition to present status and technical challenges for development new ICMs. Moreover, the key ML algorithms for ion exchange membranes (IEMs) development techniques together with available ML frameworks and their potential uses in optimization of membranes structural properties, performance prediction, and new materials discovery are discussed. The challenges and the future directional approaches to accelerate the development of robust ICMs using ML driven research that ultimately improving the sustainability and efficiency of fuel cell technologies are elaborated.

Keywords: Machine learning, ion conduction membranes, ML frameworks, fuel cells, deep learning

1.0 INTRODUCTION

The transition towards cleaner energy sources has underscored the importance of fuel cell technologies as a typical example for hydrogen utilization. Fuel cell technology is regarded as an efficient method for converting chemical energy into electrical energy, offering high conversion efficiency and reduced environmental impact. Especially, polymer electrolyte membrane fuel cells, which are suitable for wide range of applications including portable devices, mobile powertrains and stationary power generator [1, 2].

Polymer electrolyte membrane fuel cells provide significant advantages over other renewable energy sources due to their high efficiency, compact design, and ability to deliver continuous power output. Unlike solar and wind energy, which are dependent on environmental conditions, fuel cells use controlled electrochemical reactions to produce electricity, ensuring a reliable energy supply for applications requiring consistent power, such as portable electronics, automotive powertrains, and stationary power generation and backup

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systems. Their low operating temperatures enable rapid start-up and shut-down, making them highly suitable for dynamic applications where flexibility and quick responsiveness are crucial [3].

PEMFCs also offer high power density, allowing for lightweight and compact system designs, which is ideal for space-constrained applications like portable power generation and transport systems. They produce only water as a byproduct, minimizing their environmental footprint and supporting efforts to reduce greenhouse gas emissions. Moreover, PEMFCs can integrate with other renewable sources to enhance energy storage capabilities, converting excess energy into chemical energy for later use. Compared to batteries, PEMFCs tend to have longer lifespans and less performance degradation over time, making them a durable and scalable option in the push toward sustainable and resilient energy solutions [4].

1.1 Polymer Electrolyte Membrane Fuel Cells

Polymer electrolyte membrane fuel cells are devices that convert gaseous or liquid fuels into electrical energy using oxygen as the oxidant, facilitated by a catalyst, without relying on combustion processes. When hydrogen serves as the fuel, the system is classified as a proton exchange membrane fuel cell (PEMFC). For liquid fuels such as methanol, ethanol, or formic acid, the fuel cells are designated as direct methanol fuel cells (DMFCs), direct alcohol fuel cells (DAFCs), or direct formic acid fuel cells (DFAFCs), respectively. Liquid fuels simplify the design and operation of fuel cells, enabling their use in portable applications with higher energy densities. Particularly, DAFCs hold several key advantages over the more established methanol fuel cell, including a comparably high real open-circuit voltage, reduced fuel crossover through a Nafion membrane and a benign toxicological fuel profile. Figure 1 illustrates a schematic of polymer electrolyte membrane fuel cells using various fuels and their operational principles. While air can replace pure oxygen as an oxidant, adjustments in the fuel-to-oxidant ratio are necessary to counter potential declines in performance.

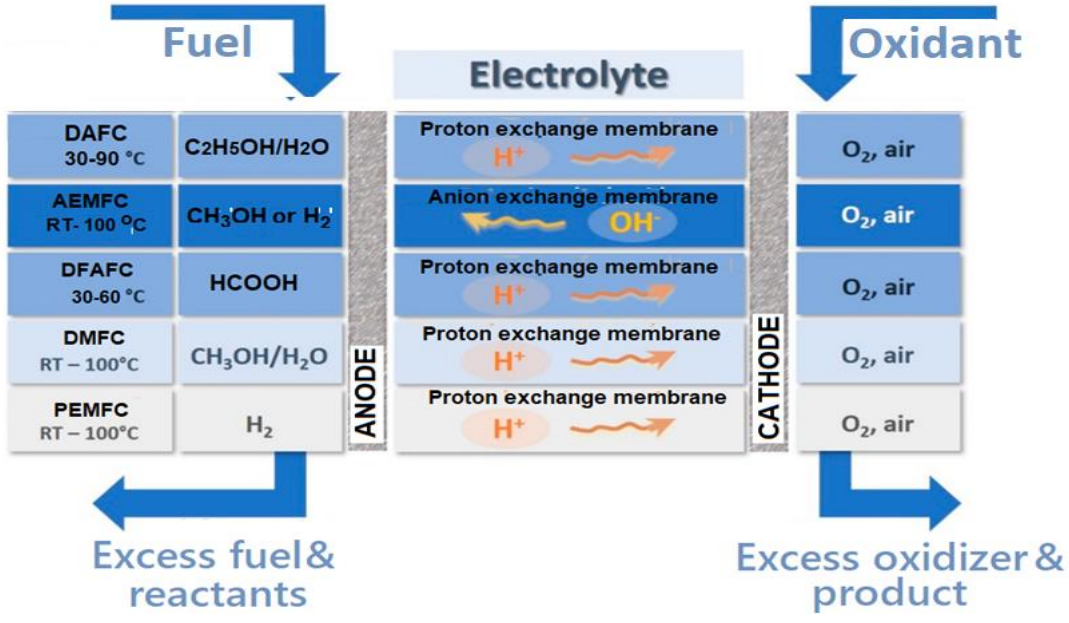

Figure 1 Schematic diagram of various polymer electrolyte membranes fuel cells

Ion conducting membrane (ICM) is a crucial component as it plays chemical function represented by ion transfer and mechanical function preventing fuel crossover. Proton exchange membranes (PEMs) conduct protons, whereas anion exchange membranes (AEMs) transport hydroxide ions and reduce fuel crossover, facilitating the use of non-precious metal catalysts in AEMFCs. To put ICM into function, it is sandwiched between an anode and cathode forming membrane/electrode assembly which is so critical for operation. Nafion®, perfluorinated sulfonic acid (PFSA) membranes, is widespread used as proton conducting membrane where FumaTech® and Aemion® are used as hydroxide conducting membranes [5]. However, the high cost of Nafion® and lack of long-term stability of FumaTech® and Aemion® (>1000 h) drive the exploration of alternative membranes [6]. Numerous research institutes are exploring novel materials with the goal of creating high ionically conductive, chemically stable, and cost-effective membranes. These efforts include innovative approaches such as blending monomers with films, incorporating crosslinkers, or using comonomers with films and formation of nanocomposite membranes [7].

1.2 Current Status and Technical Challenges for New Membranes

Majority of newly investigated advanced materials like porous frameworks, cross-linked structures, and inorganic-organic composites are being explored to overcome the limitations of conventional polymeric membranes and enhance their overall performance in fuel cell applications [8]. However, these materials face several challenges that affect their performance and commercialization. These include limited thermal stability, strong dependence on hydration for maintaining proton conductivity, and issues with fuel crossover, which reduce efficiency. Additionally, chemical degradation from exposure to highly oxidated environments, mechanical durability issues due to swelling and shrinking, and the high cost of materials like PFSA membranes pose significant obstacles [9]. While alternative materials aim to reduce costs, they often struggle to match the performance and stability of conventional options. Balancing ionic conductivity with durability and managing gas or liquid fuel permeability are critical for improving membrane effectiveness in various fuel cell applications. The required characteristics that should be enhanced in new generation of ICMs for polymer electrolyte membrane fuel cells are summarized in Table 1.

Designing high-performance membranes poses significant challenges due to the complexity of interactions at molecular and macroscopic levels. Traditional experimental approaches for discovering and optimizing new membrane materials are time-consuming and costly, often involving extensive trial-and-error. To address these limitations, machine learning has emerged as a promising approach, leveraging computational power and vast datasets to predict material properties, optimize manufacturing processes, and improve the overall performance of fuel cells [10].

Table 1 Summary of required characteristics of ICMs to enhance performance of polymer electrolyte membrane fuel cells

Requirement	Description	Target Fuel Cell Type	Refs
Selective permeability	Developing membranes that restrict fuel crossover (e.g., methanol or formic acid) while maintaining ion transport, using hybrid or multilayered structures.	DMFCs, DFAFCs	[11,12]
High proton conductivity	Incorporating polymer with high ion-exchange capacity and proton-conductive fillers like sulfonated polymers or inorganic additives to facilitate effective ion transport.	PEMFCs, DMFCs	[13,14]
High hydroxide conductivity	Incorporating polymer with high ion-exchange capacity and OH-conductive fillers with high ion conductivity over a wide relative humidity range such quaternary ammonia functionalized membrane.	DMFCs, AEMFCs	[15]
Chemical Stability	Using robust polymer backbones, such as aromatic or partially fluorinated polymers, and employing cross-linking or reinforcement techniques to enhance resistance to acidic or alkaline environments.	PEMFCs, DMFCs, DFAFCs, AEMFCs	[16,17]
Mechanical Strength	Ensuring membrane durability through the use of reinforced structures or composite designs to prevent deformation and maintain structural integrity under operational conditions.	PEMFCs, DMFCs' AEMFCs	[18,19]
Thermal Stability	Enhancing membrane stability over a range of temperatures through thermal stabilizers or adaptable microstructures to ensure consistent performance.	PEMFCs, DMFCs, AEMFCs	[20,21]
Water Management	Optimizing the balance between hydrophilic and hydrophobic regions to improve hydration, maintain high ionic conductivity, and minimize swelling.	PEMFCs, DMFCs	[22,23]
Cost Reduction	Exploring low-cost, non-fluorinated polymers as alternatives to expensive materials like Nafion, aiming for a balance between performance and affordability.	PEMFCs, DMFCs, DFAFCs, AEMFCs	[24,25]
Advanced Fabrication Techniques	Using methods like electrospinning and phase inversion to create tailored microstructures that enhance ion transport pathways and control permeability.	PEMFCs, DMFCs, DFAFCs, AEMFCs	[26,27]

1.3 Machine Learning for Development of Membranes for Fuel Cells

Machine learning (ML) can play a pivotal role in addressing the multifaceted challenges associated with fuel cell membranes by facilitating the discovery and optimization of advanced materials, hybrid membranes, and novel fabrication techniques in addition to performance prediction [28]. ML algorithms can accelerate the identification and design of materials with desired properties, such as improved ionic conductivity, thermal stability, and chemical durability. Through the analysis of large datasets and predictive modeling, ML can optimize the synthesis of porous framework membranes (PFMs), cross-linked polymeric structures, and inorganic-organic composite membranes, aiming to enhance

mechanical robustness, reduce fuel crossover, and improve ion transport mechanisms [29]. By guiding the design of these advanced materials, ML can significantly contribute to overcoming the performance limitations of traditional polymeric membranes in fuel cell applications, thus expediting the development of high-performance, cost-effective membranes. This article discusses and promotes the applications of ML in the design and prediction of ICMs design properties and performance, providing insights into how these methods can revolutionize fuel cell research.

2.0 OVERVIEW OF FUNDAMENTALS OF MACHINE LEARNING ALGORITHMS FOR IEMS DEVELOPMENT

ML which is a branch of artificial intelligence (AI) can be used to develop algorithms capable of learning from prior data and generalize their judgment to new observations by exploiting primarily statistical methods. Particularly, this learning process allows ML algorithms to construct models that capture insights derived from the data. These models are then applied to generate predictions or make decisions autonomously, without the need for predefined programming rules. ML algorithms are particularly adept at recognizing patterns and correlations within datasets, which enables them to produce accurate predictions or execute decisions when confronted with new, previously unseen inputs. This capacity for data-driven learning and generalization to novel cases is a fundamental feature of ML, underpinning its diverse applications across multiple fields [30]. ML algorithms can be classified into several categories based on their learning approach and the nature of the data as illustrated in Figure 2. The main classifications include supervised learning, unsupervised learning, reinforcement learning, semi-supervised learning, and transfer learning, each offering unique advantages for different stages of material discovery and optimization in fuel cell applications [31].

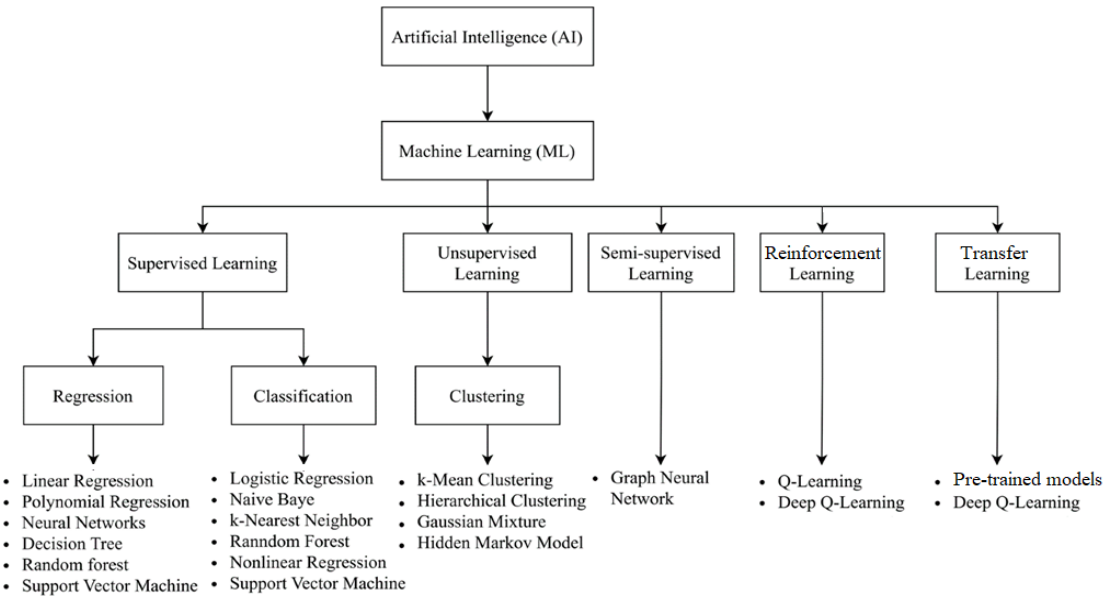

Figure 2 Classification of machine learning algorithms [31]

2.1 Supervised Learning

Supervised learning (SL) involves using labeled datasets to train models that can make predictions or classify data into categories. This approach is particularly effective in predicting material properties for fuel cell membranes, where input features (independent variables) like temperature, pressure, and chemical composition can be used to predict outputs such as ionic conductivity or chemical stability (response of dependent variable) [32]. The popular SL algorithms include Linear regression which fits a linear model based on ordinary least squares, which is common benchmark algorithm to evaluate the prediction performance of other regression algorithms. k-nearest neighbor (kNN) is another SL which is a simple algorithm that classifies a new point by a majority vote of its k nearest neighbors in the available dataset [33]. On the other hand, logistic regression is another linear model for classification rather than regression, especially binary classification. The logistic function allows the calculation of the probability of a single trail. Decision tree is another algorithm that can learn simple decision rules from data features to predict targets and can solve both regression and classification problems [34]. Naïve Bayes is another algorithm that is based on Bayes' theorem with the assumption of conditional independence between the features [35]. The support vector machine (SVM), which is based on the Vapnik-Chervonenkis dimension and structural risk minimization in statistical theory can be not only used to construct the hyperplane in a high-dimensional space to classify the samples but also it can solve regression problems, usually known as support vector regression [36]. The Gaussian process algorithm which is generic SL tool can solve both regression and classification problems [37]. Finally, Artificial neural network (ANN) represents SL algorithm that is based on modern neuroscience to process information by simulating the neural network processing in organic brains that a structure that has a multi-layer perceptron, consisting of many connected neurons [38]. A detailed review of popular supervised learning algorithms and their characteristics have been discussed elsewhere [10]. Zhang *et al*. (2020) [39] demonstrated the use of supervised learning techniques, such as support SVM and NN), for optimizing membrane materials in proton exchange membrane fuel cells (PEMFCs), resulting in improved performance prediction accuracy and reduced experimental costs.

2.2 Unsupervised Learning

Unsupervised learning (UL) differs from SL by working with unlabeled data, making it suitable for discovering hidden patterns or structures in data without predefined labels. Techniques like clustering (e.g. K-means) and dimensionality reduction methods such as Principal Component Analysis (PCA) are widely used to categorize materials based on their properties or to reduce data complexity [32]. For example, Kim *et al*. (2019) [40] applied unsupervised learning to classify material properties, facilitating the identification of promising candidate membrane materials for further development. These methods are particularly useful in early-stage research when exploring new membrane materials with unknown characteristics.

2.3 Reinforcement Learning

Reinforcement learning (RL) focuses on training agents to interact with an environment, learning strategies that maximize cumulative rewards over time. This approach is beneficial for optimizing complex, dynamic systems, such as adjusting operational conditions

in fuel cells to maximize efficiency or lifespan [41]. Lee *et al*. (2020) [42] employed RL techniques to optimize operational parameters for fuel cells, showcasing the potential of RL to enhance performance in real-time applications. RL is particularly advantageous when the performance of membranes in fuel cell system involves variables that dynamically change, requiring adaptive decision-making strategies.

2.4 Semi-supervised Learning

Semi-supervised learning (SSL) combines aspects of both supervised and unsupervised learning by using a small amount of labeled data along with a larger set of unlabeled data. This approach is effective when labeled data is scarce, which is often the case in new membrane material research [43]. Wang *et al*. (2022) [44] utilized semi-supervised learning to predict fuel cell membrane properties with limited experimental data, achieving improved prediction accuracy and reduced reliance on expensive data collection. By leveraging unlabeled data, semi-supervised learning can reduce costs associated with generating labeled datasets, accelerating the development process.

2.5 Transfer Learning

Transfer learning (TL) involves adapting a model trained on one problem to apply to a different, but related problem, which can significantly reduce the training time for new tasks. This is particularly valuable in the development of new membrane materials, where data is limited but similarities to previously studied materials exist [45]. Chen *et al*. (2021) [46] demonstrated that transfer learning could be used to adapt models trained on known membrane materials to predict the properties of new ion conducting membranes (ICMs), allowing for faster identification of high-performance materials for fuel cells.

A summary of various categories of machine learning algorithms with their applications in fuel cell membranes is listed in Table 2.

Table 2 Categories of machine learning algorithms with their applications in fuel cell membranes

Category	Definition	Common Algorithms	Applications	Refs
Supervised Learning	Learning from labeled data to map inputs to outputs.	Linear regression, SVM, neural networks, decision trees.	Property prediction, classification tasks, e.g., predicting membrane ionic conductivity.	[38,39]
Unsupervised Learning	Finding patterns in unlabeled data without explicit outputs.	K-means, PCA, t-SNE, autoencoders.	Clustering materials, feature extraction, anomaly detection in membrane data.	[40]
Reinforcement Learning	Learning through interactions with an environment to maximize cumulative reward.	Q-learning, DQN, policy gradients.	Process optimization, dynamic system control for fuel cell efficiency.	[42]
Semi-Supervised Learning	Combining small labeled datasets with larger unlabeled data.	Self-training, label propagation.	Property prediction with limited labeled data for new membrane materials.	[44]
Transfer Learning	Using knowledge from one problem to solve related problems.	Fine-tuning pretrained models, transfer of feature representations.	Adapting models for predicting properties of new membranes with limited data.	[46]

It can be observed that the cited studies illustrate the suitability of application of various machine learning techniques in the context of fuel cell membrane research, providing insights into how each method can be effectively used to address challenges in the design, optimization, and performance prediction of membrane materials. This further offers pathways to enhance efficiency, reduce costs, and expedite the discovery of novel materials. Each approach can be tailored to specific aspects of membrane design and optimization, making ML an integral part of modern fuel cell research.

3.0 PUBLICLY AVAILABLE MACHINE LEARNING FRAMEWORKS

The development of ICMs for fuel cells can benefit from a range ML frame works that are made available. Table 3 presents a list of public ML frameworks and their applications and advantages.

Table 3 List of public ML frameworks and their applications and advantages

MLTool/Framework	Type	Applications	Advantages	Refs
Scikit-Learn	Python Library	Property prediction, regression, classification, clustering of membrane materials.	Easy to use, versatile models for structured data analysis.	[47]
TensorFlow & PyTorch	Deep Learning Frameworks	DNNs for predicting membrane performance, CNNs for image-based analysis of membrane microstructure, GANs for generating new membrane designs.	Customizable architecture, suited for complex data-driven tasks.	[48,49]
RDKit & Matminer	Chemoinformatics/Materials Informatics	Feature extraction from polymer structures, virtual screening of new membrane materials, analysis of molecular structures for ionic conductivity.	Integrates chemical data with ML, detailed molecular analysis.	[54]
AutoML Tools (e.g., TPOT, H2O.ai, AutoKeras)	Automated Machine Learning	Automates model selection for optimal membrane material properties prediction, enables rapid evaluation of different ML algorithms for fuel cell performance.	Reduces manual model tuning, easier experimentation.	[51]
GpyTorch & scikit-optimize	Gaussian Processes & Bayesian Optimization	Predicting ion conductivity with uncertainty quantification, optimizing synthesis conditions for novel membranes, guiding experimental synthesis.	Effective with small datasets, probabilistic approach.	[57]
Graph Neural Networks (e.g., DGL, PyTorch Geometric)	Deep Learning for Graph Data	Models complex polymer structures and interactions, predicts membrane properties like stability and conductivity, enables discovery of novel materials.	Captures complex structural information for accurate predictions.	[53]
Materials Project, OpenMM, Quantum Espresso	High-Throughput Simulation Platforms	Provides training data for ML models, simulates atomic interactions within membranes, supports modeling of ion transport dynamics in fuel cell membranes.	Enables large dataset generation for reliable ML models.	[55]

The references cited are directly related to the application of machine learning techniques in the field of fuel cell membrane research. Each reference links to studies that employ these tools for optimizing the performance, synthesis, and characterization of membranes for fuel cell applications. Scikit-Learn, a versatile Python library, is effective for regression, classification, and clustering tasks, making it useful for predicting membrane properties like proton conductivity and stability [47]. Deep learning (DL) frameworks such as TensorFlow and PyTorch enable complex modeling through neural networks, including convolutional neural networks (CNNs) for analyzing microstructures and generative adversarial networks (GANs) for designing new materials [48, 49]. Graph neural networks (GNNs), using libraries like DGL and PyTorch Geometric, excel at representing and predicting the properties of complex polymer structures, capturing interactions at the atomic level [50]. Automated machine learning (AutoML) tools like TPOT, H2O.ai, and AutoKeras facilitate the rapid testing and optimization of various ML algorithms to predict material properties and enhance synthesis processes [51]. Bayesian optimization and Gaussian Processes, implemented through tools like GPyTorch and scikit-optimize, provide a framework for optimizing synthesis conditions and design parameters with a focus on uncertainty quantification, which is critical for guiding experimental efforts [52, 53.]. Additionally, cheminformatics and materials informatics platforms such as RDKit and Matminer are valuable for extracting features from molecular structures and integrating them into ML models [54]. High-throughput simulation platforms like Materials Project, OpenMM [55], and Quantum Espresso generate large datasets that feed into these ML models, helping to predict and optimize ionic transport and other membrane properties [56]. These tools collectively enhance the design, performance prediction, and optimization of next-generation ICMs for fuel cells.

4.0 AREAS WHERE MACHINE LEARNING CAN ENHANCE FUEL CELL MEMBRANES DEVELOPMENT

These applications demonstrate the potential of machine learning to transform the development of high-performance fuel cell membranes, addressing existing challenges and accelerating progress toward more efficient and cost-effective energy solutions.

4.1 Material Discovery and Screening

ML algorithms can predict material properties such as ionic conductivity, chemical stability [58], and mechanical strength based on molecular structures, accelerating the identification of novel membrane materials [59]. Techniques like deep neural networks (DNNs) and graph neural networks (GNNs) can model complex molecular interactions and identify candidates with optimal performance characteristics. [60].

4.2 Structure-property Relationships

By analyzing large datasets of experimental and computational results, ML can uncover hidden correlations between the structural features of polymer electrolyte membranes and their functional properties. This includes understanding how factors like

pore size distribution, crystallinity, and polymer chain flexibility affect ionic transport and membrane durability. Recent advances in deep neural networks can be employed to model these relationships effectively and accurately and to explain physics-informed DL models. The physics of two-phase transient, membrane hydration/dehydration, time constants, transport dynamics, and electrochemical double-layer behaviors can be encoded to the neural networks for effective DL [61]. Frameworks like Scikit-Learn, H_2O, and Caffe2 for machine learning and PyTorch, TensorFlow, and Keras for deep neural networks provide tools for developing these predictive models, allowing researchers to optimize membrane materials based on structural parameters. Recently, graph neural networks (GNNs) were utilized to explore the relationships between the molecular structure and properties of polymers based on supervised learning, enhancing the understanding of how modifications at the molecular level can improve performance [62, 63]. Recent research demonstrates that self-trained GNN provided more accurate prediction for membrane properties based on microstructural features [64].

4.3 Optimization of Synthesis Conditions

ML models, such as Gaussian Processes (GPs) and Bayesian Optimization, can refine synthesis parameters (e.g., temperature, time, concentration) to maximize the performance of fuel cell membranes, significantly reducing the need for extensive trial-and-error in the laboratory. For instance, GPs can model the relationship between synthesis conditions and membrane properties, offering a probabilistic approach to understanding how changes in parameters affect outcomes like membrane thickness, porosity, and ionic conductivity. By incorporating uncertainty into predictions, GPs provide a reliable means to explore the parameter space, enabling more efficient experimentation [65]. Bayesian Optimization can then use these models to identify the optimal synthesis conditions that enhance membrane performance, such as achieving a specific porosity or maintaining a uniform membrane thickness [47]. Recent research has utilized these approaches to optimize performance of fuel cell with polymer electrolyte membrane [66].

4.4 Performance Prediction under Varying Conditions

ML tools can predict the performance of membranes under different operating conditions such as temperature, humidity, and pressure, offering insights into stability and efficiency across a range of environments in fuel cells, which is crucial for assessing their viability before large-scale manufacturing. For example, Random Forest models have been used to predict proton conductivity and mechanical properties of fuel cell membranes at varying temperatures and humidity levels, providing a comprehensive understanding of their operational stability [63, 67]. Moreover, Support Vector Machines (SVM) have been applied efficiently to model performance of PEMFC with considerable reduction of the samples used in the training phase of the SVM model and allowed prediction of the voltage of the PEMFC and capturing its dynamic characteristic [68]. Furthermore, gradient boosting methods like XGBoost have been employed to predict the efficiency of fuel cells based on input features like membrane thickness and ionic conductivity, allowing for targeted optimization [69.]. On the other hand, Neural networks, such as Long Short-

Term Memory (LSTM) networks, have proven effective in forecasting performance degradation over time under fluctuating conditions and was used to develop dynamic performance of PEMFC [70].

4.5 Simulation and Modeling of Ionic Transport

ML-assisted simulations can enhance the understanding of ion transport mechanisms within polymer membranes. DL models can predict proton or hydroxide ion conductivity and diffusion pathways, supplementing traditional molecular dynamics simulations and enabling more accurate modeling of ion transport dynamics. For example, deep neural networks have been employed to predict ion conductivity in polymer membranes, using datasets from molecular dynamics simulations to train models with high accuracy [71]. These models have been implemented in frameworks like TensorFlow and PyTorch to analyze the intricate ion-movement pathways within complex polymer structures. Graph neural networks (GNNs) can also be applied to capture spatial relationships in membrane structures, aiding in the understanding of how structural features impact ion transport [72]. Additionally, Gaussian process regression models, such as those implemented in GPyTorch, have been used to refine predictions of ion mobility based on changes in temperature or pressure conditions, complementing the predictions from molecular dynamics simulations [73]. These ML/DL tools provide valuable insights that extend beyond the capabilities of traditional simulations, facilitating a more thorough understanding of ion transport behaviors in polymer electrolyte membranes.

4.6 Design of Hybrid Membranes:

ML can facilitate the design and optimization of composite or hybrid membranes that combine organic and inorganic materials to enhance thermal stability, mechanical strength, and overall conductivity. By exploring a large compositional space, ML can identify promising combinations and configurations that may be challenging to discover through traditional experimental methods. For example, Bayesian optimization models, implemented through frameworks like Scikit-learn and Optuna, have been used to identify optimal ratios of inorganic fillers such as silica or graphene oxide within polymer matrices, leading to improved mechanical properties and thermal stability [74]. Similarly, deep learning algorithms, using platforms like TensorFlow, have been applied to predict how variations in polymer blends affect the overall conductivity of hybrid membranes [75]. Gaussian process regression models have also been employed to optimize the distribution and interaction of organic-inorganic phases in hybrid membranes, aiding in the discovery of new compositions with balanced ionic conductivity and durability [76]. These ML frameworks streamline the discovery process, reducing the need for labor-intensive experimentation and accelerating the development of advanced composite membranes.

4.7 Lifetime Prediction and Degradation Analysis

One of the key challenges in fuel cell deployment is predicting the long-term durability of membranes. Degradation can occur due to mechanical stress, chemical attack, or thermal instability, impacting the membrane's performance over time. DL models trained on long-term operational data can predict degradation rates and failure modes of membranes under various conditions. For example, recurrent neural networks (RNNs), implemented through

frameworks like TensorFlow and Keras, have been used to analyze time-series data from fuel cell operation, providing insights into how operational conditions impact membrane degradation [77]. Additionally, survival models like Cox proportional hazards models can be employed to assess the probability of membrane failure over time, helping to identify the most critical degradation mechanisms [78]. This helps in designing more durable membranes by understanding the critical factors that influence their lifespan. Techniques like time-series analysis, RNNs or survival models are particularly useful in this context, allowing researchers to pinpoint operational thresholds and adjust material compositions accordingly to prolong membrane life.

4.8 Cost Reduction and Scale-up

By integrating ML with economic and environmental impact assessments, researchers can identify membrane materials and processes that balance performance with cost-effectiveness, aiding the transition from lab-scale discoveries to commercially viable solutions [79]. ML can help to develop robotic chemists resembling human features that can independently work in a standard laboratory using various apparatuses to conduct thousands of experiments that normally takes years in months allowing big datasets, which allowing completion of R&D cycle by combining this with Bayesian optimization [80]. ML can also support the scaling up of fabrication processes by predicting production challenges and optimizing resource use. For example, random forest models, implemented through frameworks like Scikit-learn, have been used to evaluate the trade-offs between membrane performance and production costs, allowing researchers to identify materials that provide the best value for specific applications [81]. Moreover, reinforcement learning approaches, utilizing platforms like TensorFlow, can optimize fabrication processes by simulating different production scenarios, thereby identifying the most efficient pathways for scaling up membrane synthesis while minimizing waste [82]. Gaussian process models, available through GPyTorch, have also been applied to predict energy consumption and environmental impact metrics during the membrane manufacturing process, helping to pinpoint areas where energy use can be reduced without sacrificing product quality [83]. These ML-driven approaches facilitate the design of economically and environmentally sustainable fuel cell membranes, ultimately bridging the gap between laboratory innovation and market-ready products.

4.9 Virtual Screening and Inverse design

With the help of ML, virtual screening can rapidly evaluate thousands of potential membrane materials, narrowing down the most promising options. Techniques such as random forests or gradient boosting are often used to rank candidate materials based on their predicted properties. For instance, Random Forest models implemented via the Scikit-learn library have been utilized to predict key properties like proton conductivity, enabling a faster assessment of potential candidates [84]. Furthermore, generative models like generative adversarial networks (GANs) or variational autoencoders (VAEs) can be applied for inverse design, suggesting new membrane structures that meet specific performance criteria. For example, GANs, using frameworks like TensorFlow, have been employed to

generate new polymer structures with enhanced ionic transport properties while maintaining chemical robustness [85]. Recent research has demonstrated the use of ML in screening a large library of polymer electrolytes, identifying candidates with high proton conductivity while maintaining chemical stability under operating conditions [86]. This approach reduced the time to identify new materials by over 50% compared to traditional methods, underscoring the efficiency of ML in the material discovery process.

4.10 Materials Discovery and Design

ML models can be trained on datasets of known IEMs to predict key properties like ionic conductivity, mechanical strength, thermal stability, and chemical resistance. This helps in identifying new materials with desirable characteristics. ML-based virtual screening of materials can rapidly identify candidates that meet specific criteria. This significantly reduces the time and cost associated with traditional trial-and-error experimental methods. Chemistry-Informed Machine Learning, which combines the principles of chemistry with advanced ML techniques can be used for polymer electrolyte discovery combines to accelerate the identification and optimization of polymer electrolytes for applications like fuel cells, electrolyzers and batteries [87]. In this approach, domain-specific chemical knowledge, such as molecular structures, bonding interactions, and reaction mechanisms, is integrated into ML models to improve their predictive accuracy and relevance [88]. For example, incorporating information about polymer chain flexibility, ion-exchange capacities, or interaction energies between polymer segments can help ML models more accurately predict properties like ionic conductivity, mechanical strength, and thermal stability [89]. This approach allows researchers to screen vast libraries of potential polymer candidates, predict their performance under different conditions, and identify optimal materials for specific applications [90]. By combining the chemical insights with power of ML that is abbreviated as CIML can reduce the need for time-consuming experimental trials, enabling faster discovery and development of advanced polymer electrolytes with desired properties (Zhang *et al*., 2020). This synergy is particularly valuable in designing materials that meet the complex performance criteria required for efficient energy conversion and storage [91].

4.11 Optimization of Manufacturing Processes

Beyond material discovery and performance prediction, ML can optimize the manufacturing processes of ion conducting membranes, enhancing their quality and consistency [92,93]. ML algorithms can analyze the effects of various manufacturing parameters such as casting thickness, curing temperature, and solvent selection on the final properties of membranes [94]. Using techniques like regression analysis or Bayesian optimization, researchers can identify the optimal set of parameters that yield membranes with the desired thickness, mechanical strength, and uniformity [95]. ML models can monitor the manufacturing process in real-time, identifying deviations or anomalies that could affect the quality of the membranes [96]. This enables predictive maintenance and quality control, reducing waste and improving yield [97]. A support vector machine

model used in membrane casting processes improved thickness consistency by 15%, leading to more reliable performance in PEMFC applications [93].

5.0 CHALLENGES AND PROSPECTIVE

The convergence of ML with fuel cell research holds the promise of unlocking new membrane materials and optimizing their performance in ways previously unimaginable. However, the current works in the open literature demonstrates a lack of DL models applications in developing more accurate results for the new membrane materials due to lack of large datasets. These large datasets are basically data collected during the monitoring of the experiment or generated via extensive simulation. Further, since these large datasets are not made public, it hinders the participation of a larger number of curious researchers and stake-holders. Furthermore, lack of standardization to data collection standard operating procedures (SOPs) and guidelines hinders gauging the accuracy of the developed models and prevents the reproducibility of the results. By accelerating the pace of discovery and enabling more efficient manufacturing processes, ML has the potential to make fuel cells a more viable and sustainable energy solution. Despite its potential, the integration of ML in membrane design and performance prediction faces several challenges. Data availability remains a bottleneck, as large, high-quality datasets are essential for training robust models. Additionally, the complexity of ML models can make them difficult to interpret, hindering the ability to gain mechanistic insights from their predictions. Future research should focus on developing more interpretable ML models, improving data sharing across research institutions, and integrating ML with high-throughput experimentation. Table 4 summarizes the primary challenges and strategic approaches to overcoming them for advancing ML-based development of ICMs for fuel cell applications.

Table 4 Summary of challenges and suggested solutions for integrating ML in the design and performance prediction of ICMs for fuel cells

Challenge	Description	Potential Solutions
Data Availability & Quality	- Large, high-quality datasets are required for training ML models, but data are often limited, fragmented, or inconsistent across studies.	- Develop open-access databases and standardized data repositories. - Encourage data sharing and collaboration across research institutions and industry. - Use high-throughput experimentation to generate comprehensive datasets.
Model Interpretability	- Complex ML models, like deep neural networks, often act as "black boxes," making it difficult to gain mechanistic insights into membrane behavior.	- Focus on developing explainable AI (XAI) methods for better insight into model decisions. - Combine data-driven methods with physics-based models to provide a more interpretable approach. - Employ hybrid models that balance accuracy and transparency.
Model Transferability	- ML models may not generalize well when applied to new materials or different operating conditions, limiting their applicability.	- Integrate domain knowledge, such as physical and chemical principles, into ML models to enhance generalizability. - Use active learning to identify critical experiments, helping models adapt to

Challenge	Description	Potential Solutions
		new conditions. - Perform cross-validation on diverse datasets.
Resource-Intensive Data Generation	- Experimental data collection can be time-consuming and costly, slowing down model development.	- Combine ML with high-throughput experimentation and computational simulations for faster data acquisition. - Use active learning to prioritize experiments that provide the most informative data. - Explore virtual screening to predict promising candidates before physical testing.
Balancing Accuracy and Physics	- ML models can be accurate but lack physical grounding, potentially leading to predictions that defy known physical or chemical laws.	- Develop hybrid models that integrate physics-based simulations with ML predictions. - Use transfer learning to apply knowledge from well-studied systems to new materials. - Regularly validate model predictions with experimental data to ensure reliability.
Scalability of Computational Models	- Scaling ML models to study complex membrane structures and performance under a wide range of conditions can be computationally expensive.	- Utilize cloud-based ML frameworks for distributed computing (e.g., TensorFlow, PyTorch). - Optimize models using dimensionality reduction techniques like PCA to focus on key features. - Employ parallel processing for computationally intensive tasks.
Lack of Deep Learning models	- ML requires manual selection of features and fingerprinting, limiting the capabilities of AI applications.	- Experimenting with several deep learning models with big datasets.
Lack of big datasets	- Utilizing deep learning for better accuracy requires large datasets but requires more computational resources.	- More initiatives are needed to generate large experimental and simulation-based datasets to facilitate the use of new and powerful deep learning models.
Lack of standardized public datasets	- Public datasets require sharing experimental and emulation data with other research groups around the globe and opens the work for more scrutiny. - Standardization efforts are long and tedious tasks and often come with conflicting interests.	- Public datasets allow for fairer and more accurate benchmarking and fine-tuning of models, while standardization exercises allow for reproducibility of results.

6.0 CONCLUSIONS

ML approaches provide a more efficient alternative transformative means by leveraging large datasets and advanced algorithms to predict membranes material properties, optimize fabrication processes, and simulate performance in fuel cells under various operating conditions. By analyzing the relationships between structural features and functional properties, ML can guide the design of new membrane materials and facilitate the discovery of novel compositions. Additionally, ML can help predict the performance of membranes in different environmental conditions, thereby enhancing the

stability and durability of fuel cell systems. ML further offers significant computation efficiency and taking into account the effects of physics that are yet unknown or formulated but contained in training databases. As a result, ML-driven methods have the potential to revolutionize the development of ICMs, making them more efficient, cost-effective, and scalable for a variety of applications, from portable devices to automotive power systems. Particularly, ML can significantly enhance the development of ICMs for fuel cell applications. This is likely to lead to and advancement in fuel cell technology by reducing the cost and improving the durability/performance. Embracing ML-driven approaches will be crucial for the next generation of high-efficiency, durable, and cost-effective fuel cells, paving the way for a cleaner energy future.

CONFLICTS OF INTEREST

The author(s) declare(s) that there is no conflict of interest regarding the publication of this paper.

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