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Data-Driven Modeling and Optimization of Polymeric Membranes for CO2 Separation: A Machine Learning Perspective

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Abstract
Polymeric membranes have become a promising technique for the reduction of greenhouse gas emissions, as they provide energy-efficient, scalable, and simple processes for the separation of carbon dioxide (CO2). Nevertheless, the design of high-performance polymer membranes is a challenging task since permeability and selectivity tend to be at odds. Recently, machine learning (ML) methods have been widely studied in order to accelerate membrane material discovery through the learning of the structure–property relationships of materials in experimental and computational data sets. This study presents a thorough survey of recent ML approaches used for gas separation material property prediction and optimization in polymer membranes. The performance, strengths, and limitations of a wide array of algorithms namely Random Forest, Support Vector Regression, Gaussian Process Regression, Deep Neural Networks, XGBoost, CatBoost are critically examined in relation to membrane properties. In addition, several challenges associated with ML applications, such as small amounts of data, model interpretability, uncertainty quantification, and generalization issues are discussed. Building on the aforementioned insights, an architecture design for solving membrane material selection problems is proposed, combining techniques such as molecular fingerprint representations, ensembles learning, interpretable ML, and uncertainty-aware screening strategies.

Keywords: *CO2 separation; Machine learning; Membrane Optimization; Polymeric Membranes; Uncertainty quantification.*

1. Introduction

Climate change is an issue that develops because of increasing amounts of greenhouse gases in the atmosphere and is one of the major problems that confronts humans today. In these greenhouse gases, CO2 is considered the key factor behind climate change, which is released due to fossil fuel combustion, manufacturing activities, power generation, and transport movements (Dangayach et al., 2025). Hence, there is an urgent need for the development of carbon capture and gas separation technologies to achieve environmental sustainability. There are several gas separation technologies that have been utilized, which include absorption, adsorption, cryogenic distillation, and membrane separation, among others (Dangayach et al., 2025). Out of all these technologies, the method of gas separation using membranes has emerged as a preferred choice, mainly because it requires minimal energy, simple operations, compactness, and scalability. In addition, the use of polymeric membranes is becoming more popular because of the advantages associated with these membranes such as their relatively low costs, mechanical robustness, ease of manufacture, and ability to be implemented on a large scale. Two main metrics used for evaluating the performance of polymeric membranes include permeability and selectivity. The former is associated with the speed with which gases diffuse across a membrane, while the latter describes the membrane's efficiency in separating different types of gases. Nevertheless, there is a fundamental limitation in designing polymeric membranes, known as the permeability-selectivity trade-off, which is popularly referred to as Robeson Upper Bound (Robeson, 2008). In general, discovering new membrane materials has been a process involving experimental studies. While such an approach yields reliable results, it is costly, time-consuming, and labor-intensive (Barnett et al., 2020). Moreover, the extensive chemical space that polymer materials occupy makes experimental screening a challenging task. Consequently, modern approaches for designing polymeric membranes tend to incorporate computational techniques to reduce development costs. The recent advancements in Artificial Intelligence (AI) and ML technologies can be considered promising tools when creating membranes using data analytics (Pan et al., 2022). Besides being able to discover complex interactions between different molecular characteristics and membrane properties, ML models allow one to predict various aspects of the membrane's performance very accurately. Among the most successful types of ML models in the field, there are Support Vector Regression (SVR), Random Forest (RF), Gaussian Process Regression (GPR), Deep Neural Network (DNN), XGBoost, and CatBoost. In recent years, researchers have developed even more sophisticated methods of membrane property prediction and selection, such as molecular fingerprints, graph learning, explainable artificial intelligence (XAI), uncertainty quantification, and multi-objective optimization. However, some issues persist that require solving, namely insufficient amount of available data, poor explainability of models, uncertainties associated with predictions, scalability problems, and the absence of integrated frameworks. This review offers a thorough examination of ML-based techniques for polymeric membrane modeling and optimization in the application of CO2 separation processes (Basdogan et al., 2024; Yang et al., 2022; Ochiai et al., 2025). First, basic concepts related to the process of membrane gas separation are introduced; then, existing approaches to the development of ML models for predicting membrane properties are presented and discussed. Current challenges related to membrane modeling and optimization are addressed, and a comparison of available approaches is offered. Finally, an intelligent framework for accelerating membrane discovery based on ML, XAI, and optimization methods is suggested. In what follows, the organization of the rest of this article can be outlined as follows. Section II describes the basics of carbon dioxide separation and polymeric membranes. Section III covers ML methods employed in modeling and predicting membrane behavior. Section IV describes a comparative evaluation of different methodologies that exist in the literature. Section V identifies the research gaps and challenges. Section VI proposes an intelligent approach [1-5].

2. Fundamentals of Co_2 Separation and Polymeric Membranes

2.1. CO_2 Separation Technologies

The rising amount of CO2 in the atmosphere has led to increased interest in methods of gas separation that can be used for effective CO2 removal. Methods such as absorption, adsorption, cryogenic distillation, and membrane separation have been developed for CO2 capture, where the former two employ liquid or solid sorbents, respectively, while the latter uses differences in boiling points of gases (Dangayach et al., 2025; Xu et al., 2024). Of these technologies, membrane separation is increasingly gaining popularity due to the relatively low amount of energy used, smaller scale of equipment required, ease of operation, and scalability. In this method, gas molecules are separated by differences in the permeability coefficients of gases. The use of membrane separation for various industrial purposes is thus becoming more widespread.

2.2. Polymeric Membranes

The polymeric membranes are the semi-permeable materials that have the ability to selectively permeate certain gases and block others (Zentou et al., 2026; Thajudeen et al., 2026). The polymeric membranes are widely applied in gas separation operations due to their low cost, easy manufacture process, high mechanical strength, and ease of scaling up the process (Glass et al., 2024; Xu et al., 2024). The polymers used to make these membranes include polysulfone, polyimide, cellulose acetate, and polyethylene oxide polymers. Such materials are widely applied in various industrial processes including natural gas purification, hydrogen

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production, oxygen enrichment, and carbon dioxide removal (Dangayach et al., 2025). The efficiency of separation by polymeric membranes is dependent on the molecular structure of the polymer and gas-membrane interactions. However, polymeric membranes tend to face the problem of a trade-off between permeability and selectivity (Robeson, 2008). Therefore, substantial research is currently dedicated to developing highly efficient membranes.

2.3. Performance Metrics: Permeability and Selectivity

The performance of polymer-based membranes is usually measured based on two main factors: permeability and selectivity. Permeability refers to the speed at which the molecule of gas can pass through the membrane. This parameter determines the efficiency of separation processes because high permeability allows for quick movement of molecules and small membrane areas. The selectivity is related to the preference of membranes for the particular species of gas. In the case of CO_2/CH_4 separation, the membrane with high selectivity will enable more CO_2 molecules to permeate and fewer CH_4 molecules to pass. High permeability and high selectivity are desired properties of any membrane; however, it is difficult to combine them in one membrane.

2.4. Robeson Upper Bound

The difficulty in designing polymeric membranes lies in the balance between permeability and selectivity, also referred to as the Robeson Upper Bound (Robeson, 2008). In most cases, polymeric membranes that have high permeability properties are relatively less selective, and those that are highly selective lack permeability properties. The inability to develop membranes that are highly permeable and selective is attributed to this balance in membrane design, making it difficult to achieve both gas permeation and gas separation through membranes.

2.5. Need for Machine Learning in Membrane Design

The design and optimization process of polymeric membranes usually depends on experimentation that is usually costly, tedious, and time-consuming (Abdollahi et al., 2025). Additionally, because there are too many polymer molecular structures to screen through experimentally, the whole process becomes difficult. The use of ML algorithms makes this process easier because it allows one to quickly predict properties of the materials based on the available data from experiments and simulations (Abdollahi et al., 2025). In addition, it allows us to find the relationship between the molecular structures of the materials and their performances in gas separation [6-10].

3. Machine Learning Techniques for Polymeric Membranes

ML is increasingly proving to be efficient in modeling membranes and developing high-performing polymer-based membranes. Through training the model on intricate relationships between material structure and gas-separating properties, it becomes possible to achieve huge savings in time and labor. Many ML techniques have been used in predicting membrane properties, each exhibiting its own strengths and weaknesses.

3.1. Traditional Machine Learning Techniques

Some conventional techniques employed for gas permeability and selectivity prediction include SVR, RF, and GPR. The SVR technique proves to be effective at dealing with small datasets as it allows for modeling of nonlinear relations based on kernel learning techniques. RF is known for its resistance to overfitting, while being efficient at processing high-dimensional molecular descriptors (Hao et al., 2025; Xu et al., 2024). In turn, GPR yields not only predictions but also provides an estimate of the uncertainty of the model, thus becoming useful for membrane screening tasks. Nonetheless, there might be some limitations associated with these techniques.

3.2. Deep Learning Methods

A number of deep learning methods have received significant recognition because of their ability to automatically learn features from data. DNNs can capture complicated non-linear interactions and provide better results when adequate amounts of training data are present (Dangayach et al., 2025; Glass et al., 2024). More recently, GCN and GIN were used to learn information from graph structures of molecules. Even though deep learning methods can give good predictions, they are known to need huge amounts of data, and they do not provide enough transparency [11-15].

3.3. Ensemble Learning Methods

The approach to ensemble learning makes use of

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multiple learning models to obtain more accurate and robust predictions (Sallam et al., 2025). Algorithms such as RF, XGBoost, and CatBoost have exhibited impressive results in predicting membrane properties. The algorithms are known for their ability to address nonlinearities, high-dimensionality, and structure-property interaction. In addition, boosting algorithms have often outperformed traditional regression algorithms in terms of prediction accuracy. Nonetheless, ensemble algorithms usually require careful tuning of parameters and give little physical understanding regarding the process of gas transport through membranes. In conclusion, the use of ML algorithms holds immense promise for the prediction of membrane properties and materials screening. Further efforts are still needed owing to several limitations that have emerged in the field. The summary of the most common ML methods that are employed for polymeric membranes modeling is presented in Table 1. Their main advantages, drawbacks, and application examples are listed there.

Table 1 Comparison of ML Techniques for Polymeric Membrane Modeling

ML Method	Strengths	Limitations	Applications
SVR	Effective for small datasets	Parameter sensitive	Gas permeability prediction
RF	Robust and interpretable	Limited uncertainty estimation	Membrane-property prediction
GPR	Provides uncertainty estimates	Computationally expensive	Membrane screening
DNN	Learns complex nonlinear patterns	Requires large datasets	Property prediction
XGBoost	High prediction accuracy	Complex tuning	Material optimization

Table 2 presents some selected ML models from the latest scientific literature on polymeric membranes and discusses the applicability, prediction accuracy, and shortcomings of each.

Table 2 Comparison of Representative ML Approaches for Polymeric Membrane Modeling

Ref.	Model	Application	Performance	Limitation
(Barnett et al., 2020)	GPR	CO_2/CH_4	$R^2 = 0.875$	Small dataset
(Yang et al., 2022)	DNN	CO_2/CH_4	$R^2 = 0.900$	Low interpretability
(Pan et al., 2022)	SVR	CO_2/CH_4	$R^2 = 0.841$	Parameter sensitive
(Basdogan et al., 2024)	RF	CO_2/N_2, CO_2/O_2	$R^2 = 0.937$	No uncertainty analysis
(Xu et al., 2024)	GCN, GIN	O_2/N_2, H_2/CH_4, and H_2/N_2	MAE = 0.461	High complexity
(Ochiai et al., 2025)	GPR	CO_2/N_2, CO_2/CH_4	$R^2 = 0.939$	Limited screening

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(Zentou et al., 2026)	RF, XGBoost	CO_2/N_2, CO_2/O_2, CO_2/H_2	MAE= 346.92 Barrer	No feasibility study
(Glass et al., 2024)	Gradient Boost	Membrane property prediction	MAE= 122.0 LMH/bar	Small dataset

As depicted in Table 2, ML methods have exhibited potential success in terms of predicting membrane characteristics as well as their ability to separate gases. Methods such as ensemble learning like RF and XGBoost usually exhibit high predictability accuracy, while deep learning and graph neural networks manage to recognize structural-property relations. Nevertheless, some issues like dataset scarcity, lack of explainability, no uncertainty measurement, and computational complexity still pose barriers for their implementation in membrane engineering [16-20].

4. Comparative Analysis and Discussion

However, despite substantial advancements in ML modeling of polymeric membranes, differences in performance among various models depend significantly on the dataset used and prediction goals, which leads to specific issues affecting the success rate of ML models used in predicting membrane properties.

4.1. Reasons for Superior Performance of Ensemble Learning

The models utilizing ensemble learning, such as RF and XGBoost, frequently exhibit better predictive ability than classical models for membrane property prediction (Sallam et al., 2025). The reason for better model performance in this case lies in the fact that, in contrast to other ML approaches, these models are capable of handling nonlinear dependencies between molecule descriptors and properties of interest without overfitting the model. Moreover, models based on ensemble learning can manage high dimensionality associated with fingerprints. Nevertheless, these types of models suffer from high complexity in parameter setting and lack interpretability.

4.2. Data Scarcity and Dataset Limitations

Performance of ML techniques heavily relies on having an adequate amount of high-quality training data (Nasef & Habaebi, 2025). Due to the expensive nature of manufacturing and analysis of membrane materials, experimental datasets in the field are rather scarce. The presence of variations in testing conditions may also lead to noise generation during data collection and preprocessing stages. These limitations prevent model generalization and can affect its accuracy while making predictions about previously unseen samples.

4.3. Lack of Explainability

Deep learning and ensemble methods are known to provide good prediction accuracy (Sallam et al., 2025). At the same time, they could be viewed as black box models that complicate explaining the importance of certain molecular features and their effect on properties such as permeability and selectivity. Therefore, research interests are shifting towards interpretable AI.

4.4. Generalization and Scalability Problems

While many ML techniques show excellent results when making predictions using previously seen membrane datasets, they often fail to predict properties of entirely novel polymer structures. Moreover, high computational costs involved in screening thousands of materials may pose another issue that requires solving. The following Table 3 describes some of the main problems encountered when applying ML models for polymeric membranes along with the appropriate solutions.

Table 3 Major Challenges in ML -Based Polymeric Membrane Modeling

Challenge	Impact on ML Models	Current Approaches
Data Scarcity	Poor generalization	Data augmentation, transfer learning

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Interpretability	Black-box predictions	SHAP, Feature Importance
Uncertainty	Low prediction reliability	GPR, Bayesian methods
Scalability	Slow screening	Ensemble learning, optimized algorithms

5. Research Challenges and Gaps

Despite many advancements in the application of ML for the gas separation through polymer membranes, some scientific gaps persist as seen in Figure 1. According to the findings of the literature review, the following gaps need to be addressed:

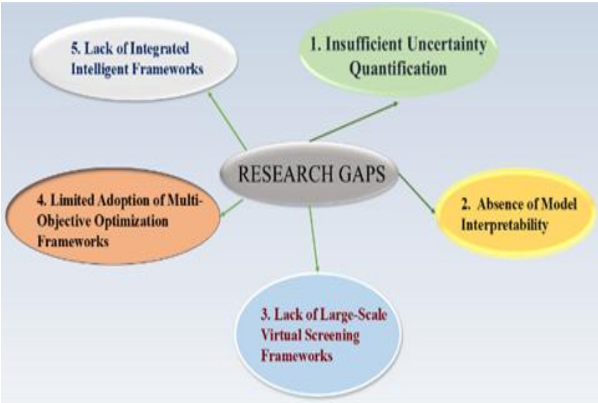

Figure 1 Research Challenges and Gaps in ML-Based Polymeric Membrane Design

5.1. Insufficient Uncertainty Quantification

A majority of the current studies tend to concentrate on improving the prediction quality in terms of R2, RMSE, and MAE. However, only a few research papers address uncertainty quantification, and this hinders the assessment of the prediction reliability for new polymer materials. Reliable uncertainty estimation is vital in practical membrane screening.

5.2. Absence of Model Interpretability

Modern methods for membrane screening include DNN, GNN, as well as boosting-based approaches. These models are considered black boxes because they lack interpretability (Ricci & De Angelis, 2023; Talukder et al., 2024). Despite the high quality of the predictions obtained by modern approaches, there is no information about the structure that determines permeability and selectivity of a membrane.

5.3. Lack of Large-Scale Virtual Screening Frameworks

Although many studies have shown effective prediction accuracy, a very small number of research works are available with an emphasis on large scale virtual screening for polymer membranes (Xie et al., 2025). Screening framework that allows quick identification of suitable material from extensive design space is necessary.

5.4. Limited Adoption of Multi-Objective Optimization Frameworks

Current ML methods mainly aim at improving one objective function while ignoring the other one. In contrast, membrane design requires consideration of both permeability and selectivity simultaneously because of their intrinsic tradeoff, which is captured by Robeson upper bound. While there exist research studies considering multi-objective optimization methods, their implementation in membrane informatics still needs improvement. Therefore, frameworks addressing multiple objectives as well as finding optimized membranes are necessary.

5.5. Lack of Integrated Intelligent Frameworks

Most of the studies in the literature have been dealing with single objectives such as prediction, optimization, interpretation, and uncertainty quantification. It should be noted that few studies attempt to incorporate all these elements in a framework. This indicates that most of the approaches proposed so far do not offer end-to-end solutions for membrane discovery and screening. In order to resolve this problem, a complete solution approach is discussed in the next section.

6. Proposed Intelligent Framework

In order to bridge the research gaps that have been observed in existing studies, an intelligent framework using ML techniques is introduced for the development and optimization of polymer membranes as depicted in Figure 2. The proposed framework involves several components such as feature extraction, modeling, explainable artificial intelligence, uncertainty quantification, and multi-objective optimization. In contrast to traditional methods that are concerned only with prediction accuracy, the novel intelligent framework pays attention to factors such as prediction reliability,

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interpretability, and intelligent candidate selection.

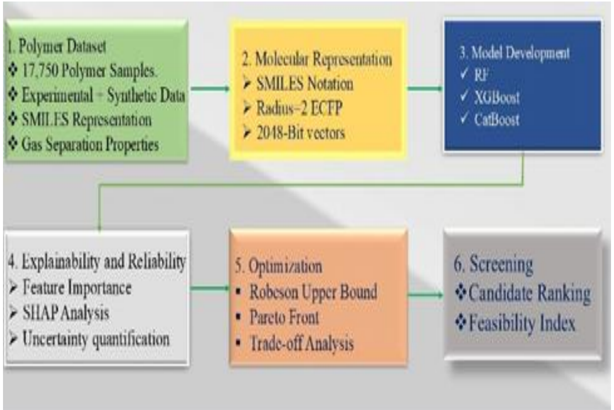

Figure 2 Proposed Intelligent Framework for ML-Based Polymeric Membrane Design

The suggested framework starts with acquiring the information on polymer membrane through experiments, literature reports, and computationally designed polymer membrane systems. Molecular structures are encoded via SMILES notation and then converted into Extended Connectivity Fingerprints (ECFPs) for fixed-length numeric representation of their structural information (Rogers & Hahn, 2010). Such a feature extraction approach is useful to capture the essential structural information required for ML algorithms to understand the structural factors affecting gas transport through polymer membranes. After obtaining molecular descriptors, they can be passed to the prediction model that includes RF, XGBoost, and CatBoost algorithms. These algorithms will learn the membrane properties, including CO2 permeability and selectivity. To enhance the efficiency of the models, the prediction model plays a crucial role in the framework by learning the structure–property relationships between polymer molecular descriptors and membrane performance metrics. For the purpose of increasing the predictability and transparency of our proposed model, the framework also integrates XAI and uncertainty quantification methods. By performing Feature Importance and SHapley Additive exPlanations (SHAP) analyses, we are able to identify the important molecular descriptors and analyze the contribution made by each feature to the final prediction made by our model. While doing so, we simultaneously use uncertainty quantification methods to assign prediction confidence values to the results. This way, researchers are better equipped to differentiate the reliable predictions from those which should be taken with caution. Our framework further uses optimization and screening methods to examine the predicted properties of membranes. By applying the Robeson upper bound analysis and Pareto optimal candidate search strategies, the permeability-selectivity dilemma is addressed and good potential candidates are identified. Further, the screening level analysis provides us with the ranking of candidate membranes based on their performance, prediction confidence, and practicality. Our framework yields high-performing polymer membrane candidates useful for CO2 separation processes.

7. Future Research Directions

Even after achieving impressive progress in the realm of membrane design via ML algorithms, there is still considerable room for improvement in this field. This includes, among others, the exploration of state-of-the-art deep learning frameworks such as GNN and Transformers, which are capable of discovering better molecular representations compared to traditional ML methods. The next area that can be considered a research priority concerns the design of ML frameworks based on physical insight, thus integrating domain knowledge and physical laws within the modeling process. Autonomous learning and discovery of membrane material are other promising areas of study that will help in future research regarding membranes. In such cases, ML algorithms can continuously learn what type of experiments to perform so that cost savings and accelerated identification of high-performing materials can be achieved. Combination of robot learning with ML may further facilitate self-sustaining systems for membrane designing. Finally, future research on ML and membrane separation of CO2 should include the aspect of sustainability, which may involve techno-economic studies, power requirement, and environmental impact. Such inclusion can prove useful for designing ML frameworks in membranes. Moreover, other new approaches like foundation models, physics-aware deep learning, and autonomous labs may also speed up the design and development of next-generation membranes.

Conclusion

In this survey, a review of the use of ML to develop polymeric membranes for CO2 separation was comprehensively discussed. First, the basic principles of membrane gas separation were elaborated upon, including permeability, selectivity, and the Robeson upper bound to create a background for evaluating the performance of polymeric membranes. Second, different approaches of ML, such as traditional ML, deep learning, and ensemble learning, were discussed regarding their merits, limitations, and capabilities to predict membrane properties. Then, by comparing the different types of membrane property prediction, some difficulties in developing new membranes, namely the scarcity of data, poor interpretability, uncertainty in prediction, and lack of scalability, became apparent. In addition, potential research gaps in membrane informatics were identified as a result of the challenges. Finally, an intelligent framework incorporating the use of molecular fingerprint representation, ML CO2 model training, explainable AI, uncertainty estimation, and optimization was proposed in order to tackle the aforementioned challenges and promote more reliable and rapid membrane discovery. Potential future directions included advancements in graph learning, physics-informed ML, active learning, and material discovery.

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References

[1]. Abdollahi, F., Khosravi, A., Karagöz, S., & Keshavarz, A. (2025). A systematic review of recent advances in the application of machine learning in membrane-based gas separation technologies. Applied Energy, 381, 125203. https://doi.org/10.1016/j.apenergy.2024.125203

[2]. Barnett, J. W., Bilchak, C. R., Wang, Y., Benicewicz, B. C., Murdock, L. A., Bereau, T., et al. (2020). Designing exceptional gas-separation polymer membranes using machine learning. Science Advances, 6(20), eaaz4301. https://doi.org/10.1126/sciadv.aaz4301

[3]. Basdogan, Y., Pollard, D. R., Shastry, T., Carbone, M. R., Kumar, S. K., & Wang, Z.-G. (2024). Machine learning-guided discovery of polymer membranes for CO_2 separation with genetic algorithm. Journal of Membrane Science, 712, 123169. https://doi.org/10.1016/j.memsci.2024.123169

[4]. Dangayach, R., Jeong, N., Demirel, E., Uzal, N., Fung, V., & Chen, Y. (2025). Machine learning-aided inverse design and discovery of novel polymeric materials for membrane separation. Environmental Science & Technology, 59(2), 993–1012.

[5]. Glass, S., Schmidt, M., Merten, P., Abdul Latif, A., Fischer, K., Schulze, A., Friederich, P., & Filiz, V. (2024). Design of modified polymer membranes using machine learning. ACS Applied Materials & Interfaces, 16(16), 20990–21000. https://doi.org/10.1021/acsami.3c18805

[6]. Hao, S., Wang, M., Guan, H., Zhao, Y., Ji, Z., & Dai, C. (2025). Machine learning-guided prediction of polymeric membrane performance in forward osmosis. Separation and Purification Technology, 379(Part 2), 135037. https://doi.org/10.1016/j.seppur.2025.135037

[7]. Nasef, M. M., & Habaebi, M. H. (2025). Machine learning for accelerating development of ion conducting membranes for fuel cell applications. Journal of Applied Membrane Science & Technology, 29(1).

[8]. Ochiai, H., Nagai, K., & Kaneko, H. (2025). Machine learning-driven design of sustainable polymer membranes: Integrated prediction of gas permeability, selectivity, and biodegradability. ACS Omega, 11(1), 1935–1944. https://doi.org/10.1021/acsomega.5c10251

[9]. Pan, Y., He, L., Ren, Y., Wang, W., & Wang, T. (2022). Analysis of influencing factors on the gas separation performance of carbon molecular sieve membrane using machine learning technique. Membranes, 12(1), 100. https://doi.org/10.3390/membranes12010100

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Page No: 4591 - 4599
https://irjaeh.com
https://doi.org/10.47392/IRJAEH.2026.0602

[10]. Ricci, E., & De Angelis, M. G. (2023). A perspective on data-driven screening and discovery of polymer membranes for gas separation, from the molecular structure to the industrial performance. Reviews in Chemical Engineering, 40(5).
[11]. Robeson, L. M. (2008). The upper bound revisited. Journal of Membrane Science, 320(1–2), 390–400. https://doi.org/10.1016/j.memsci.2008.04.030
[12]. Rogers, D., & Hahn, M. (2010). Extended-connectivity fingerprints. Journal of Chemical Information and Modeling, 50(5), 742–754. https://doi.org/10.1021/ci100050t
[13]. Sallam, D., Shaheen, B. S., & Allam, N. K. (2025). Machine learning guidelines for designing next-generation nanocomposite membranes for CO_2 capture. Journal of Membrane Science.
[14]. Talukder, M. J., Alshami, A. S., Tayyebi, A., Ismail, N., & Yu, X. (2024). Membrane science meets machine learning: Future and potential use in assisting membrane material design and fabrication. Polymer Reviews, 64(1), 216–229. https://doi.org/10.1080/15583724.2023.2212295
[15]. Thajudeen, K. Y., Ahmed, M. M., & Alshehri, S. A. (2026). Separation process modeling and analysis in water purification based on membrane technology using artificial intelligence models. Journal of Saudi Chemical Society, 30, Article 8.
[16]. Xie, C., Qiu, H., Liu,L., You, Y., Li, H., Li, Y., et al. (2025). Machine learning approaches in polymer science: Progress and fundamental for a new paradigm. SmartMat, 6(1), e1320. https://doi.org/10.1002/smm2.1320
[17]. Xu, J., Suleiman, A., Liu, G., Perez, M., Zhang, R., Jiang, M., et al. (2024). Superior polymeric gas separation membrane designed by explainable graph machine learning. Cell Reports Physical Science, 5(7), 102067. https://doi.org/10.1016/j.xcrp.2024.102067
[18]. Xu, J., Suleiman, A., Liu, G., Zhang, R., Jiang, M., Guo, R., et al. (2024). Transcend the boundaries: Machine learning for designing polymeric membrane materials for gas separation. Chemical Physics Reviews, 5(4), 041311. https://doi.org/10.1063/5.0205433
[19]. Yang, J., Tao, L., He, J., McCutcheon, J. R., & Li, Y. (2022). Machine learning enables interpretable discovery of innovative polymers for gas separation membranes. Science Advances, 8(29), eabn9545. https://doi.org/10.1126/sciadv.abn9545
[20]. Zentou, H., Issa, M. A., Alshareef, B. S., & Abdelnaby, M. M. (2026). Practical prediction of gas separation performance in polymeric membranes using machine learning. Chemistry – An Asian Journal, 21(4), e70645. https://doi.org/10.1002/asia.70645