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A critical review on machine-learning-assisted screening and design of effective sorbents for carbon dioxide (CO_2) capture

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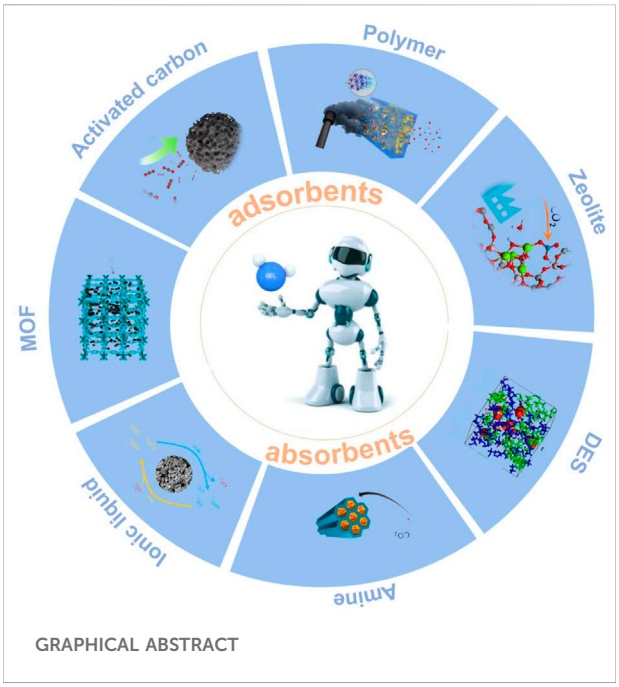
Effective carbon dioxide (CO_2) capture plays indispensable roles in closing the global carbon cycle, serving the sustainable production of energy, and achieving the grand 1.5 °C goal by 2050. Considering the diversity and complexity of CO_2 capture materials, machine learning has stepped into this field years ago and become a powerful tool that promotes the screening and design of involving parameters. From these perspectives, this critical review firstly summarizes the technical backgrounds for the applications of ML-based methods in CO_2 capture. Then, through categorizing the materials into two major groups, that is, adsorbents (containing metal organic frameworks, carbonaceous materials, polymers, and zeolites) and absorbents (involving ionic liquids, amine-based absorbents, and deep eutectic solvents), the applications of this effective tool in relevant areas are scrutinized. The major concerns remain to be further addressed are derived based on the above discussions, namely 1) the development of consistent and integrated databases, 2) the wise digitalization of inherent properties of materials, and 3) the validation of the accuracy of ML-derived results under practical scenarios. The main purpose of this critical review is bridging the previous achievements and further developments of ML-assisted design of CO_2 capture techniques.

KEYWORDS

CO2, carbon capture, machine learning, metal organic framework, flue gas

Introduction

Fighting against climate change, with emphasis on the over-accumulated issue of carbon dioxide (CO_2) in the air, is one of the most predominant challenges facing carbon-intensive energy industries and the environmental community in the 21st century (Guan et al., 2022). Compared to preindustrial times before the 1750 s, the CO_2 concentration in the troposphere has increased from ~280 ppm to ~400 ppm, with an annual increase of approximately 1 ppm (Pera-Titus 2014; Oschatz and Antonietti 2018). Notably, this increasing trend is accelerating in the past decades, with the rate boosting from ~1.1% in the 1990 s to ~3.0% in the 2000 s. The over-accumulated CO_2 in the air is escorted by the rise of Earth's surface temperature by 0.6–0.7 C (Pera-Titus 2014). Although future trends



GRAPHICAL ABSTRACT

are difficult to be specified due to unexpected geological activities, the Paris Climate Agreement identifies that, to achieve the grand 1.5°C goal, a net-zero emission of CO_2 must be realized by 2050, because even assuming a preferred scenario, the CO_2 will exceed 550 ppm until then (Wang et al., 2011). Besides, by converting it back to energy storage materials (Wu et al., 2021), adopting it in extracting residual oils from aquifers (Chen et al., 2022), *etc.*, the centralized control of CO_2 also serves the overall benefits of energy production in a depleting era of fossil fuels. From these perspectives, it is of great urgency to develop advanced and effective techniques for CO_2 capture and collection from industrial flue gas and ambient environment.

The up-to-date applications of CO_2 capture technologies generally involve an absorption process, with the addition of amine-based solution like monoethanolamine (MEA), diethanolamine (DEA), or methyl-diethanolamine (MDEA), to convert CO_2 into carbonate solids (Ghanbari et al., 2020). However, the low selectivity of traditional amine-based absorbents towards CO_2 capture remains yet a critical issue impeding the closing of carbon-cycle and the achievement of net-zero CO_2 emission (Haider and Kumar, 2020). Specifically and firstly, for CO_2 capture from industrial flue gas, the limited selectivity makes traditional amine-based absorbents efficient for the capture of components other than CO_2, e.g., sulfur dioxide (SO_2) and nitrogen oxides (NO_x), thus the separation of carbon-laden energy storage products becomes relatively time-consuming and expensive that requires extra steps (Rezaei and Jones 2014). Secondly, for the direct CO_2 capture (DAC) from ambient environment, a critical technique to achieve the net-zero emission of CO_2, using amine-based absorbents, if not being purposefully functionalized, is generally unpractical (Barzagli et al., 2020). The advancements in CO_2 capture with more functional agents exhibiting higher selectivity thus still hinder the world to be on the right track towards forming a batch of available technologies applicable under all possible scenarios.

To realize a highly selective CO_2 capture from industrial flue gas or ambient environment, advanced materials including modified amine absorbents (Pakzad et al., 2020; Gaikwad et al., 2021; Li et al., 2021; Mehrabi et al., 2022), MOFs (Ding et al., 2019), metal salts (Hu et al., 2019; Hu et al., 2021), zeolites (Khoramzadeh et al., 2019; Bakhtyari et al., 2020), deep eutectic solvents (Ali et al., 2016; Zarei et al., 2020), *etc.*, have been proposed to be alternatives to traditional CO_2 capture agents. The adjustment of physical and chemical properties of absorbents or adsorbents is the most crucial process to make them purposefully functionalized (Rahimi et al., 2021). However, considering the complex composition of the properties that can be designed, experimental methods based on a trial-and-error logic are extremely time-consuming and hardly leverage all key properties. To overcome this research gap and identify more selective agents for CO_2 separation, machine learning (ML) has been emerging as an efficient way recently, because it can screen tens of thousands of materials with a variety of physical and chemical properties being adjustable (Fernandez et al., 2014; Anderson et al., 2018; Zhu et al., 2020; Zhang et al., 2021a).

From the abovementioned perspectives, the prediction of the physical and chemical properties of CO_2 sorbents is a fundamental towards the design of functionalized CO_2 sorbents. Fortunately, using ML-based methods to characterize the inherent properties like density (Abdollahzadeh et al., 2022), viscosity (Bakhtyari et al., 2022), and pore structure (Jablonka et al., 2020) of materials has been in a developed stage. With this advancement, the foreseeable wide application of ML methods in CO_2 capture is expected to bring about revolutionary changes that extend the material reservoir, boost the sorption capacity, increase the CO_2 selectivity, and reduce the operation cost. While most previous works focused on the CO_2 uptake capacity, the CO_2 selectivity, another critical factor influencing the applicability of CO_2 capture techniques, is much less investigated and clarified, representing the bottleneck at the current stage. Considering the effectiveness of ML in identifying and proposing highly selective CO_2 ab-/adsorbents, the use of this method innovatively fuels the break of this bottleneck, but well-constructed framework bridging its previous achievements and further development in this specific field is still lacking (Zhou K. et al., 2019).

Correspondingly, this review aims to prioritize the role of selectivity in CO_2 separation from other gas components, if applicable, or discuss the future endeavors towards such a sophisticated end. It firstly and briefly introduces the technical backgrounds of ML methods. The technical backgrounds primarily include four sub-sections, that is, the collection of data, the featurization of descriptors, the

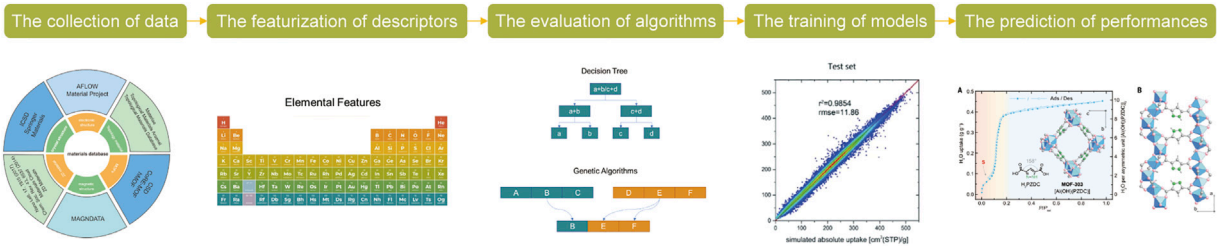


FIGURE 1
A diagrammatic illustration on the process of ML.

evaluation of algorithms, and the training of models and the prediction of performances. Then, the application of ML methods in CO_2 capture was summarized based on different kinds of materials, which can be primarily divided into adsorbents and absorbents. Adsorbents take advantage of the abundant pores, large surface area and other properties to capture CO_2, including metal organic frameworks (MOF), carbonaceous materials, polymers, and zeolites. Absorbents capture CO_2 by chemically reacting with it, including amine-based absorbents and ion-liquid based materials. Finally, the critical research gaps and future development of ML methods in related areas are identified, aiming to provide a dedicatedly constructed framework guiding the effective use of ML techniques in mitigating climate change and saving energy penalty before they step towards losing control.

Technical backgrounds

Since its appearance in the 19th century, ML has been rapidly evolving and widely used in the identification and proposal of novel materials (Lu et al., 2017; Ramprasad et al., 2017; Wang et al., 2022a; Zhang X. et al., 2022). The intelligent nature of ML methods makes it not only an efficient tool to preprocess and analyze data, but also an advanced way to learn and recognize patterns. After the sorption behaviors of CO_2 on a designated group of materials are determined using appropriate ML approaches, the CO_2 separation performances of ab-/adsorbents that have not been experimentally tested can be predicted based on this recognized pattern. Generally, the following steps represent a typical roadmap to process the ML-based design of CO_2 capture materials, that is, the collection of data, the featurization of descriptors, the evaluation of algorithms, the training of models, and the prediction of performances (Chen et al., 2020) (as briefly illustrated by Figure 1).

The collection of data. Firstly, for a ML-based task, sufficient quantity and satisfactory quality of data, which can be collected from published literatures or self-generated through theoretical calculation or experimental test (Butler et al., 2018), are the most critical factors influencing its feasibility. With approximately 40,000 referred results if using 'CO_2 capture' and 'CO_2 separation' as keywords for searching on the Web of Science, it is totally possible for ML-based studies in related areas to collect data from previous works. While the consistency of the collected data is difficult to be well-controlled, e.g., different works conducting the CO_2 capture experiments under varied conditions that may significantly change the performances, ML may be an effective method to exclude the impacts of these external factors, or even to identify the patterns of how these factors influence the CO_2 capture efficiency. In this case, these external factors must be taken as necessary descriptors and participate in the model training process. By processing importance analysis, the model tells users whether these external factors play crucial or marginal roles in the CO_2 separation process (Guan et al., 2022). If a crucial role is identified, the specific effects of experimental conditions can be investigated in detail *via* ML-based approaches, and if a marginal role is found, the experimental conditions can be generally excluded in the subsequent prediction of CO_2 capture performances. However, as the primary goal of most ML-based explorations is examining potential materials instead of practical operation conditions, self-generated data may be preferred to ensure their integrity and consistency. The Grand Canonical Monte Carlo (GCMC) method based on molecular dynamics with the assistance of density functional theory (DFT) calculation is a common roadmap to this end. This method is generally applicable in the cases where porous materials that physiosorbed CO_2, e.g., MOF, are adopted (Dureckova et al., 2019). Besides, databases like Materials Project (Jain et al., 2013), Cambridge Structural Database (Groom and Allen 2014), Crystal Open Database (Gražulis et al., 2009), *etc.*, that contain tens of thousands of known materials with necessary properties specified, which is still unceasingly updating, also build an indispensable bridge for the self-generation of data.

The featurization of descriptors. The featurization of descriptors refers to a process where essential properties

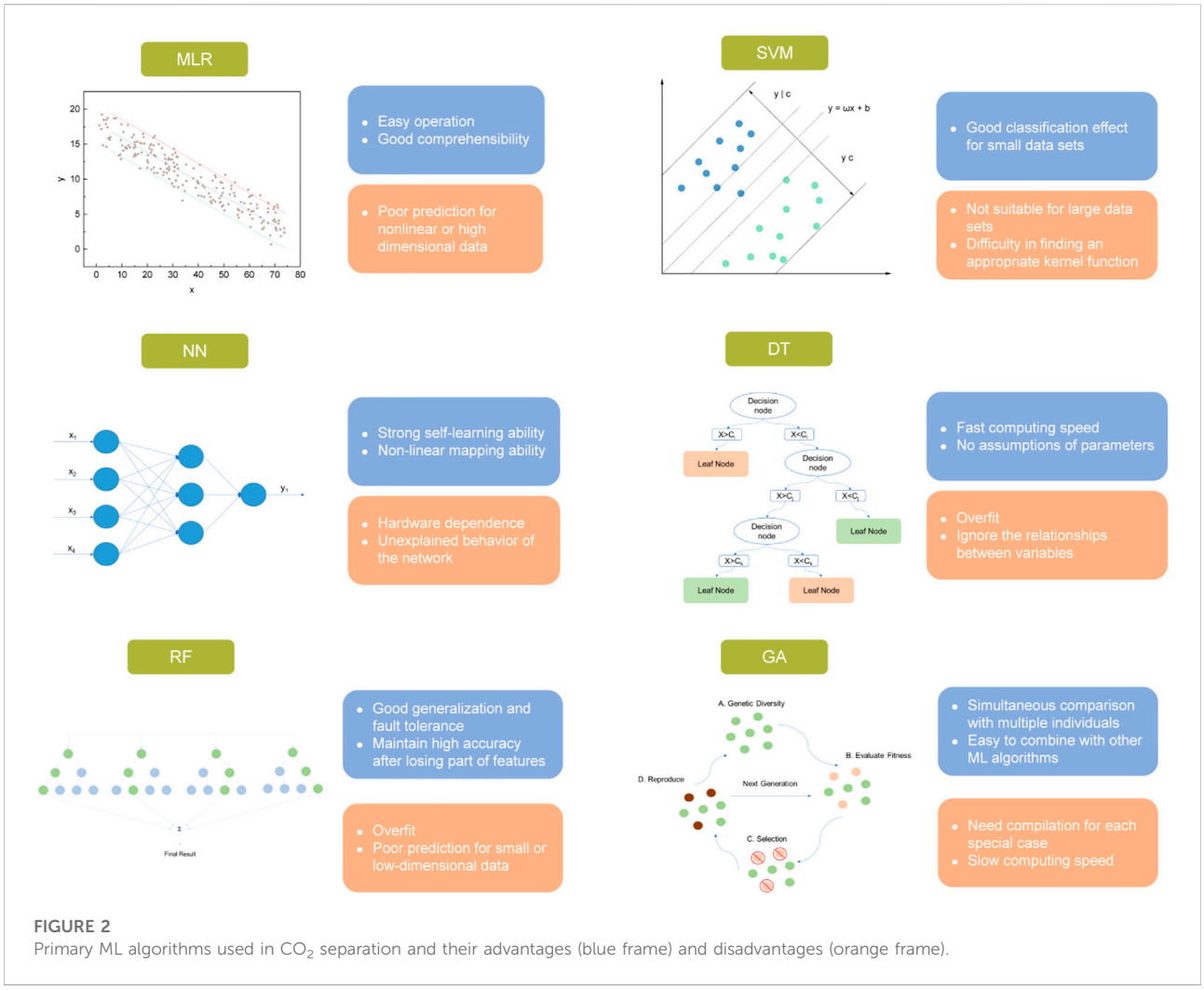


FIGURE 2
Primary ML algorithms used in CO_2 separation and their advantages (blue frame) and disadvantages (orange frame).

involved in CO_2 capture are transferred into numerical values (called descriptors) that are readable for computer. Generally, the essential properties can be categorized into two subsets, that is, external properties of experiments (e.g., the operation temperature/pressure, the concentration of CO_2, the dosage of ab-/adsorbents, *etc.*) and intrinsic properties of materials including their apparent compositions (e.g., elemental composition, the ratio between active adsorbents and inert supporters, *etc.*), physical characteristics (e.g., pore size, surface area, *etc.*), and chemical characteristics (e.g., the interaction pattern among different atoms, the charge of active sites, the d-band center of active sites, *etc.*) (Ghiasi et al., 2019; Burns et al., 2020; Shi et al., 2020; Gupta and Li 2022; Situ et al., 2022). The selection of properties is a subtle but critical task that directly determines the performance of modeling. The involved properties need to fully represent a group of possible influential factors affecting the CO_2 capture performance, while redundant inclusion of properties may cause deviation and overfitting. For example, the surface area and pore volume of a material is generally interconnected, thus the inclusion of both these two properties contain redundant information that may result in overfitting. Although this overfitting concern may be properly addressed with the use of advanced algorithms, it is better to exclude excessively interconnective data when featuring descriptors. Besides, it should be noted that, while part of the abovementioned features are numerical values in nature (e.g., the operation temperature/pressure, the pore size, and surface area), other features like the interactive pattern among different atoms may be unreadable characteristics for computers in their initial forms. For these properties, how to efficiently transfer them into numerical value is still an open question nowadays. Common methods include the use of topologically repeating units, matrix, and/or function to represent the complex situation (Behler and Parrinello 2007; Huang and von Lilienfeld 2016; Barnett et al., 2020). In addition, there are numerically-in-nature properties may proportionally correlate with those that are difficult to be digitalized. A typical example is that the

interactive pattern among different atoms may be correlated with the electronegativity of these atoms, hence users can replace the hardly-digitalized characteristics by numerically-in-nature features if their interconnective pattern is recognized to improve the efficiency and avoid overfitting.

The evaluation of algorithms. There are generally three kinds of ML - supervised learning, unsupervised learning, and reinforcement learning (Kargbo et al., 2021). Supervised learning refers to a ML scenario where both the input descriptors and output values in the training set are given, and the purpose of learning is correlating the input and output data with relatively complex laws (Tabor et al., 2018). As for unsupervised learning, unlabeled input descriptors were involved, that is, the output values remaining unclarified in this case, and the primary goal of learning in this case is recognize the patterns of data (Chen et al., 2015). Finally, reinforcement learning is a method that computer mimics the behaviors of human and improves its own ability in the learning process (Podryabinkin and Shapeev 2017). For CO_2 capture, supervised learning is the most common technique used in previous studies, and it contains different algorithms, for which the performance is case-dependent. The involved algorithms for exploring the CO_2 separation performances of different materials mainly include multiple linear regression (MLR), genetic algorithms (GA), support vector machine (SVM), decision tree (DT), random forest (RF), and neural network (NN) (with the advantages and disadvantages of each algorithm specified in Figure 2).

For effective CO_2 separation, the properties of the materials and experiments might be used as the input features, and the output values were CO_2 capacity, capture efficiency, and/or selectivity. Although the selectivity is the most concerned issue in this review, the CO_2 capacity and capture efficiency are non-neglectable in most cases as they are the foundations for an exceptional selectivity. To judge the accuracy of ML simulations, loss functions are adopted with the assistance of correlation coefficient (R^2), mean absolute error (MAE), mean square error (MSE), and root mean square error (RMSE) (Doreswamy et al., 2020). For example, a RMSE value higher than 0.80 is generally taken as a criterion to justify the applicability of a ML algorithm, and that higher than 0.90 indicates an excellent accuracy. Algorithms with higher accuracy was selected for a large-scale simulation, while inherent reasons accounting for such an empirical superiority may be complicated and unknown.

The training of models and prediction of performances. After the algorithms are optimized, it is the time to process ML learning and find the intrinsic correlations between input properties and output values. The collected data are randomly separated into two different groups namely training set and testing set in the training process of models (the size ratio between the training and testing sets generally ranges between 75%:25%–85%:15%), aiming to verify the generalization of the applied algorithms. Multiple cross validation may be in further need if the data size is relatively small (Lu et al., 2017). When, typically, RMSEs of the training and testing processes larger than 0.90 and 0.80 are obtained, it demonstrates that the descriptors adopted and the model used are suitable for the further prediction of CO_2 separation performances of untested materials (Barnett et al., 2020). The prediction only requires the input of unlabeled data with specified features and unknown performance. Descriptors that are found to have negligible influence on the performance based on the importance analysis results can be excluded from the input set in the performance prediction, if preferred. It is thus an efficient way to exclude the impact of external factors and investigate the influence of intrinsic characteristics of materials even no consensus is reached among experimenters to provide data generated under a consistent condition. A specific criterion is expected to judge the suitability and applicability of CO_2 ab-/adsorbents under practical scenarios, which generally involves the participation of the following parameters, that is, the CO_2 capacity, the CO_2 selectivity over other gas components, and the plot of CO_2 permeability *versus* its selectivity when a membrane is used (as shown in Figure 3) (Barnett et al., 2020). Tens of thousands of materials that have not been experimentally synthesized and tested can be screened in this process with a relatively high accuracy. Only the preferential materials as indicated by the ML modeling might be synthesized in some cases to further support the validation of the simulation (Zhang Z. et al., 2022), thus significantly saving the time of conducting time- and labor-consuming tests.

Application of ML in CO_2 separation

The ML based screening and design of CO_2 separation ab-/adsorbents leverage its function in the case where complicated material properties or process characteristics remain to be adjusted. According to the function of materials, they are categorized into two major parts namely adsorbents, including metal organic frameworks (MOF), carbonaceous materials, polymers, and zeolites, and absorbents, including ionic liquids (IL), amine-based materials, and deep eutectic solvents (DES) (as shown in Figure 4). It should be noted that the primary purpose of this critical review is to explore the fundamentals and applications of the ML-assisted methods in designing CO_2 capture materials, but not to give a comprehensive introduction to all available materials/techniques nowadays.

Adsorbents

***Metal organic frameworks* (*MOF*).** MOFs are one of the most explored groups for CO_2 capture based on ML-based methods. Critical reasons accounting for such popularity include 1) wide interests - the huge reservoir, theoretically

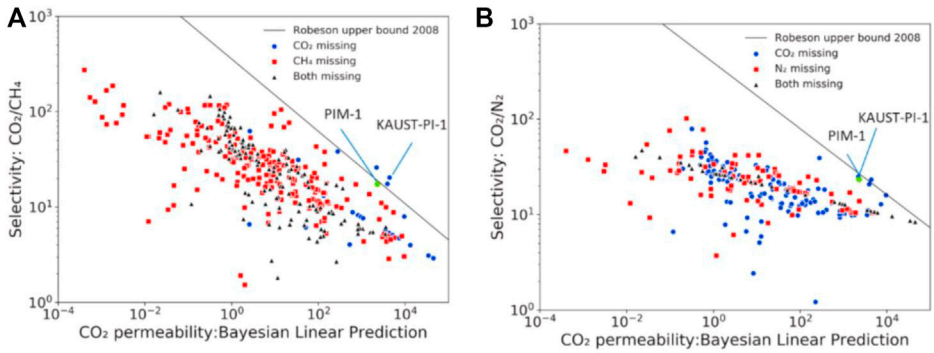


FIGURE 3
The plot of CO_2 permeability versus its selectivity over **(A)** CH_4 and **(B)** N_2 of (Yuan Q. et al., 2021).

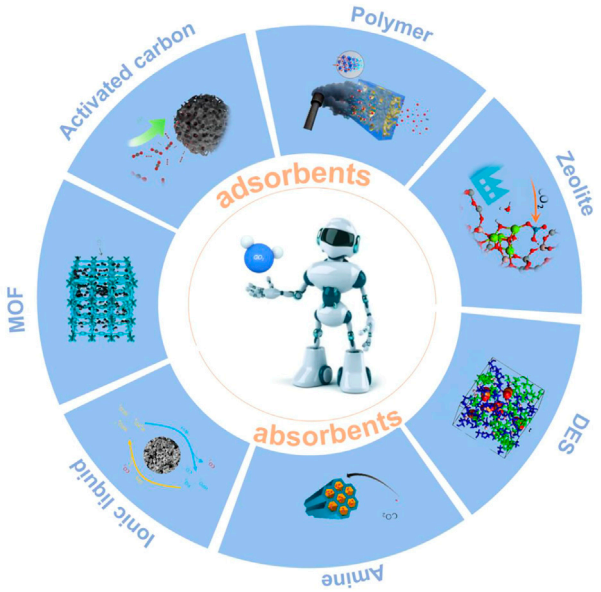


FIGURE 4
Different categories of materials used for ML-based CO_2 capture study.

infinite, of available MOFs comprised of profoundly adjustable parameters, 2) data availability - there are several databases like Cambridge Crystallographic Data Centre (CCDC) and Computation-Ready, Experimental (CoRE) containing sufficient data of experimentally synthesized and hypothesized MOFs, and 3) time and labor-saving technical roadmap - compared with experimentally testing the CO_2 adsorption capacity of MOF, computational methods (e.g., GCMC) generally spend much less time and labor costs to finish the same job. As the key influential factors affecting the physisorption, the pore sizes, surface areas, and void fractions of MOFs, experimentally accessible or derived from theoretical calculation with designated software (e.g., Zeo++), are generally included in the training of ML models. Besides, the chemical properties of MOFs are also important for the CO_2 capture, including the heat of adsorption, the atomic weight ratio of different elements, the types of metal nodes, *etc.* Although the digitalization of the chemical properties of MOFs is generally more complex than that of the physical properties, a recent work employed a GCN method to digitalize MOF structure and obtain its chemical features efficiently (Wang et al., 2022b).

The application of ML in MOF-assisted CO_2 capture dates back to 2014 when its use was for the first time reported in related areas (Fernandez et al., 2014). The SVM ML model was adopted to screen and recognize the CO_2 adsorption patterns and behaviors over more than 32,000 types of MOFs. Specific criteria were set to select the outperforming MOFs out under different operational pressures, that is, MOFs with capacities higher than 1 mmol g^{-1} at 0.15 bar and 4 mmol g^{-1} at 1.0 bar were identified as superior MOFs for CO_2 capture. Based on these criteria, a critical interatomic distance in the compact framework ranging between 6 and 9 Å was found to be optimal for CO_2 capture. An inferior interatomic distance compromised the adsorption performance probably attributed to the incapability to accommodate CO_2, while an excessive distance might allow CO_2 to bypass the adsorbents instead. In 2016, the same research group considered more than one kind of gas components and for the first time investigated the selectivity towards CO_2 over CH_4 of MOFs based on the DT and SVM ML models (Aghaji et al., 2016). It was also found that, due to a similar reason as abovementioned, moderate surface area, void fraction, and pore diameter are both important to enhance the selectivity of MOFs towards CO_2 over CH_4. A void fraction lower than 0.27 and a pore diameter lower than 6.6 Å were identified to be two critical thresholds to achieve a CO_2/CH_4 selectivity of >10. However, these two valuable works, despite shedding the initial light on the application of ML in CO_2 capture based on MOFs,

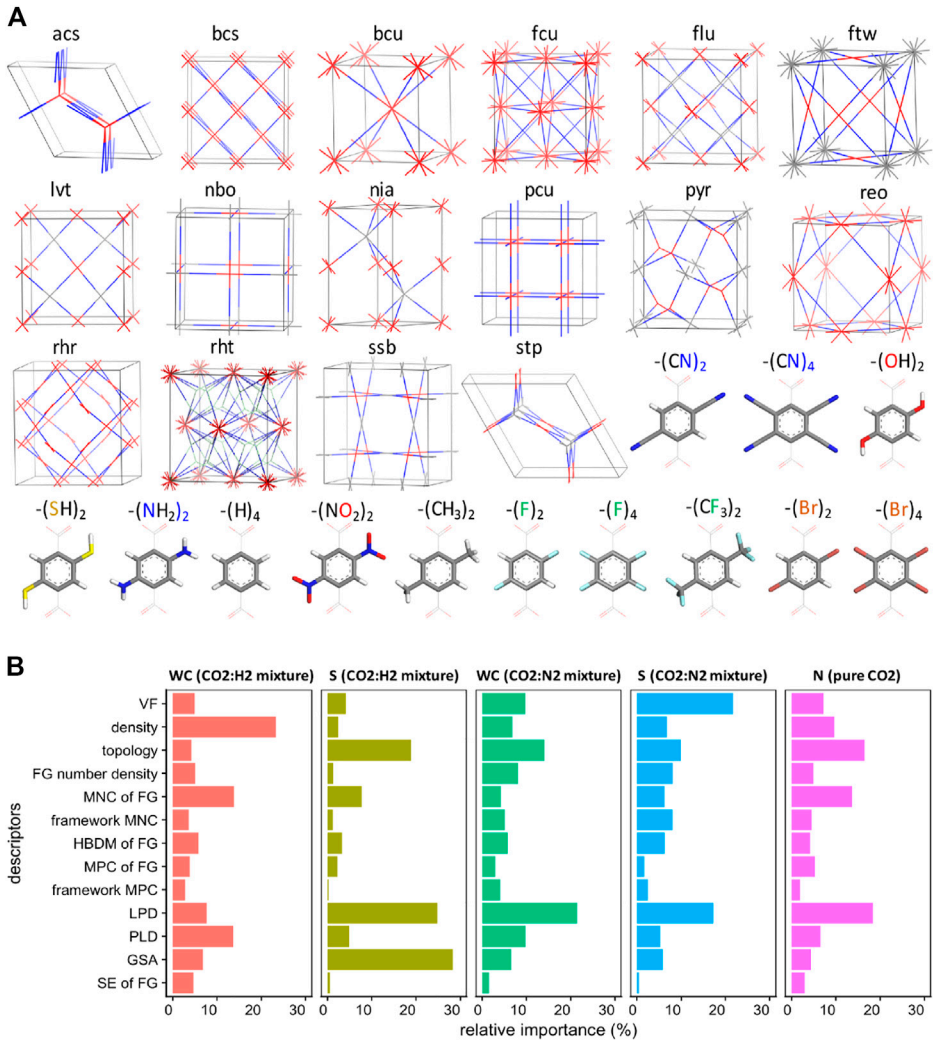


FIGURE 5
(A) Topological blueprints and connecting molecular building blocks used in the construction of the over 400 MOF designs, and **(B)** Relative importance of material descriptors obtained from GBM training (S = selectivity, WC = working capacity, N = adsorption loading. FG = functional group, VF = void fraction, HDBM = highest dipole moment, MPC = most positive charge, MNC = most negative charge, LPD = largest pore diameter, PLD = limiting pore diameter, SE = sum of epsilons, GSA = gravimetric surface area) (Anderson et al., 2018).

are deficient in nature due to the omission of their chemical properties.

To overcome such deficiency, the chemical features of MOFs were originally considered in 2018 with the assistance of a topological method (Anderson et al., 2018). The Coulomb charge of MOFs, the most positive and most negative charges in functional groups, the highest bond dipole moment of MOFs, and the topology of functional groups are involved in the model training (as shown in Figure 5A). Before introducing a crucial chemical descriptor, i.e., the topology of functional group, into the system, the authors first validated the applicability of such descriptor. Specifically, the authors adopted DFT calculation to obtain the binding energy of CO_2 on different functional groups. Then, it was found that the GCMC-derived CO_2 adsorption capacity of different MOFs was correlated with the binding energy of CO_2 on the functional groups these MOFs contain. The result demonstrated that the features of functional groups significantly influenced the CO_2 adsorption capacity of MOFs, thus they must be properly included, after digitalized, in the input set to conduct the ML study. Gradient boosted machine and NN are found to be the most accurate models to correlate these descriptors, the abovementioned chemical together with physical ones, with the CO_2 capture performances of MOFs. The simulation results showed that, although the chemical features had been included in this study, the physical characteristics like the pore size, void fraction, surface area, and density are still the

dominant influential factors affecting the working capacity of MOFs towards CO_2 capture in most cases (as shown in Figure 5B). However, for the selectivity of CO_2 over other gas components like N_2 or H_2, the topology of functional groups in MOFs did matter, indicating that the selectivity of MOFs might be more sensitive to the chemical features of MOFs than the capacity. Desired topological structures derived from the simulation results were bcs, bcu, and fcu (as shown in Figure 5A), while the inherent mechanisms accounting for such superiority remains to be further explored.

With the physical and chemical descriptors for the MOF-based CO_2 capture being proposed, from then on, studies started to investigate the performance of MOF under practical scenarios. The performance of various MOFs for CO_2 separation in the presence of water vapor was examined using a NN ML model (Zhang et al., 2021b). Both the physical and chemical features were considered in this case. The simulation results suggested that MOFs with moderate surface area (1750 $m^2 g^{-1}$) and pore diameter (14.2 Å) exhibited an optimized CO_2 separation performance if water vapor exists. The applicability of MOFs in direct CO_2 capture from air was explored based on RF, NN, DT, and SVM ML models by co-considering the influence of N_2 and O_2 (Deng et al., 2020). The heat of adsorption was found to be the most important parameter changing the CO_2 capture performances of MOFs. It should be noted that the heat of adsorption is a systematical reflection of the chemical properties of MOFs, and the specific chemical features influencing the capture performance remains unspecified. The best-performing MOF with a CSD code of NORGOS possessed a selectivity of CO_2 over N_2 + O_2 of 4712, much superior to the optimal MOFs as identified by experimental pathways. This significant outperformance further supports the unique advantage of ML-based methods in screening and designing CO_2 capture agents, while the accuracy of the adsorption capacity and CO_2 selectivity are not necessarily in accordance with their experimentally-determined ones. To further consider the real-world conditions, an industrial vacuum swing adsorption (VSA) system was adopted to evaluate the CO_2 separation performances of different MOFs from industrial flue gas (Burns et al., 2020), aiming to well-bridge the gap between material optimizations and process designs. The MOF namely ppn-6-CH2DETA was found to possess the highest selectivity towards CO_2, which exceeded 50,000 according to the GCMC calculation results. However, IISERP-MOF2, UTSA-16, and zeolite NaA, rather than ppn-6-CH2DETA, were identified to be preferred in this case with parasitic energy of lower than 250 kWh_e per MT CO_2 and productivities greater than those of pilot-scaled zeolite-13X. These results implied that, in real-world practices, in addition to the adsorption capacity and CO_2 selectivity, there are more complicated factors to be included to justify the applicability of MOFs for CO_2 separation, which remains yet to be fully clarified.

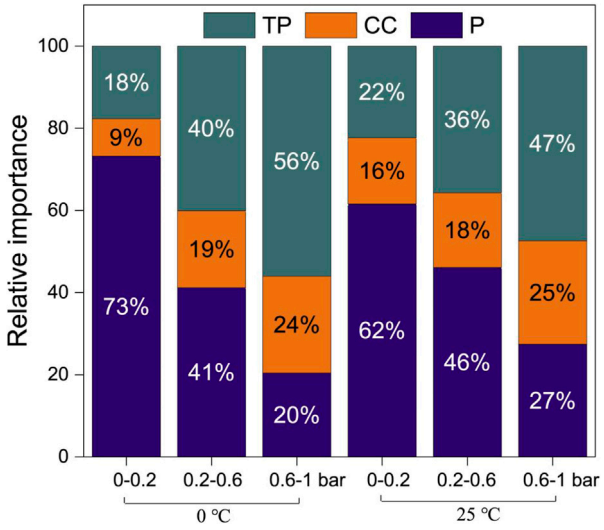


FIGURE 6
The relative importance of integrated influential factors at different pressure ranges (TP, CC and *p* represented textural properties, chemical compositions and pressure, respectively) (Zhu et al., 2020).

Carbonaceous materials. Activated carbons, attributed to its porous structure and diversified active ligands, are used for the capture of various environmental pollutants like CO_2 (Li and Xiao 2019; Sreńscek-Nazzal and Kielbasa 2019), volatile organic compounds (VOCs) (An et al., 2019; Zhou T. et al., 2019; Li et al., 2020), hazardous metals (Karnjanakom and Maneechakr 2019; Yang et al., 2019; Zhang et al., 2021c), *etc.* The relatively low unit price, the easy accessibility, the adjustable structure of pores, and the potential to be regenerated make activated carbons promising alternatives to amines for CO_2 capture under real-world conditions. Using carbonaceous materials to capture carbon becomes a popular topic nowadays through synthesizing activated adsorbents from biomass wastes. How to prioritizing the effects of different influential factors, that is, the external factors, the physical features of materials, and the chemical characteristics of adsorbents, has become a debating topic recently, and this was the time ML-based methods stepped into this specific area years ago.

To elucidate the influential importance of different types of factors on the CO_2 capture performance of activated carbons, several representative descriptors belonging to external factors (temperature and pressure), the physical features of materials (surface area, micropore volume, mesopore volume, and ultra-micropore volume), and the chemical characteristics of adsorbents (the mass percentages of hydrogen, oxygen, nitrogen, and carbon) were featured (Zhu et al., 2020) and processed based on RF model. As shown in Figure 6, the

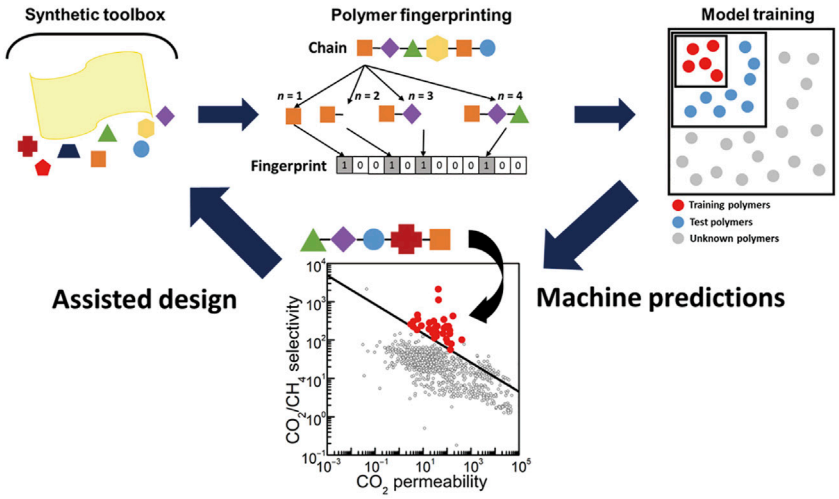


FIGURE 7
Assisted design of high-performance polymer membranes (Barnett et al., 2020).

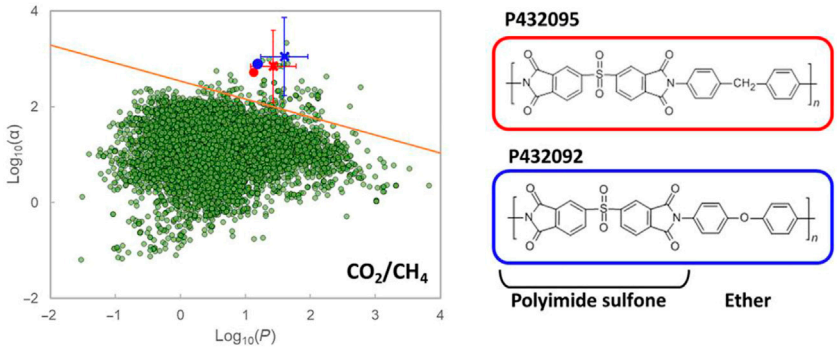


FIGURE 8
Polymer candidates for advanced CO_2/CH_4 gas transport performance identified through ML and their experimental performance (Barnett et al., 2020).

authors found that, within a low-pressure range (0–0.6 bar), pressure primarily affected the CO_2 capture performances of activated carbons, while within a high-pressure range (0.6–1 bar), the physical properties of activated carbons dominated. This phenomenon is probably attributed to that 1) microporous and ultra-microporous structures were dominated in these porous carbon materials, and 2) at high pressure, CO_2 adsorption on porous carbons proceeded through pore-filling mechanism rather than layer adsorption (Sevilla et al., 2013; Boyjoo et al., 2017). Besides, the authors also found that under a relatively low but unchanged pressure (<0.2 bar), the mesopore volume significantly influenced the CO_2 adsorption capability of activated carbons, whereas the ultra-micropore volume took this role over if the pressure increased to >0.6 bar. Although the limited sample size of this study might induce the deviation in the judgement of the role of different features, this work still offered valuable references that inspired further studies in related areas.

In 2021, the CO_2 capture performances of activated carbons were simulated and studied by different tree-based ML algorithms including gradient boosting decision tree (GBDT), light gradient boosting machines (LGB), and extreme gradient boost (XGB) (Yuan X. et al., 2021). GBDT was proven to marginally outperform other 2 ML algorithms in the simulations, and the importance of different types of descriptors follow the order external factors > physical features > chemical characteristics,

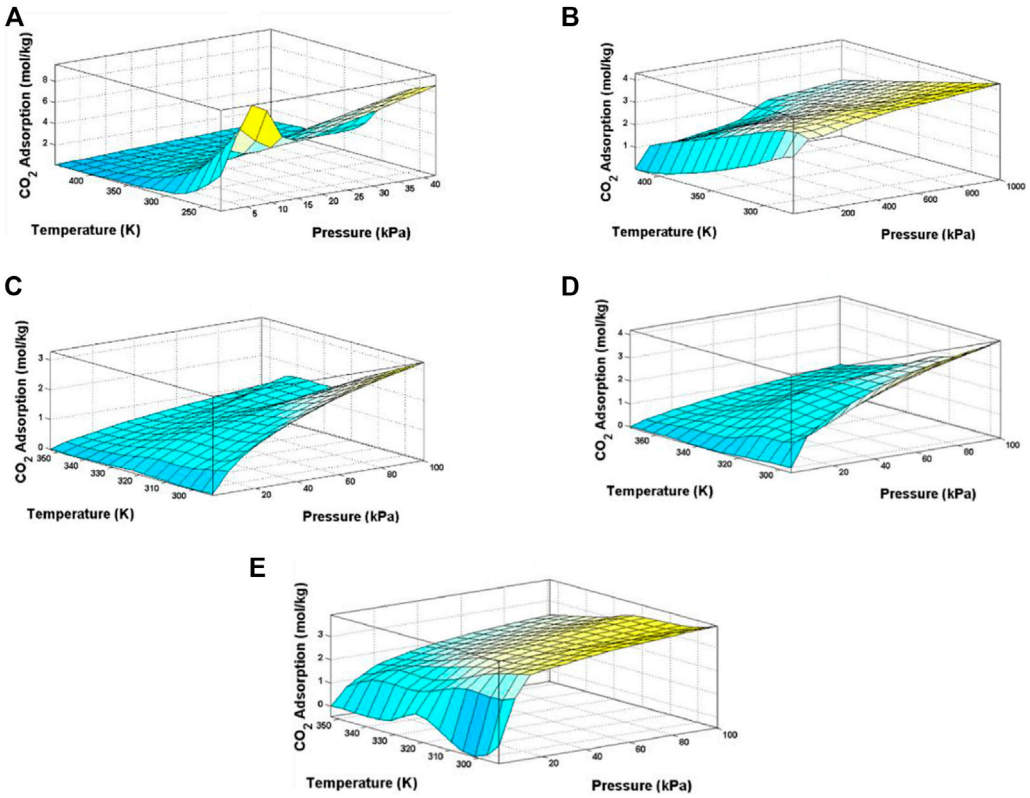


FIGURE 9
Effect of Temperature and pressure on CO_2 adsorption (axial Z) on various types of zeolite **(A)** 13X, **(B)** 5A **(C)** SAPO-34 **(D)** SSZ-13 and **(E)** T-Type (Raji et al., 2022).

which was generally in line with previous studies. The CO_2 adsorption behaviors of bio-derived N/O-enriched activated carbons were also simulated by a NN-based algorithm, and density functional theory (DFT) calculations were adopted as a supportive method to identify the adsorption mechanism of CO_2 (Rahimi et al., 2022). The role of different characteristics, that is, pyridinic nitrogen (N-6), pyrolytic nitrogen (N-5), oxidized nitrogen (N-X), graphitic nitrogen (N-Q), and the fraction of N-6/N-X, of N-containing functional groups was identified, evidencing that N-6, N-5, and N-X considerably functioned in the CO_2 capture. The CO_2 capture by rice husk derived activated carbons was studied by a NN-based algorithm, while only physical properties like pore volumes and surface areas of activated carbons were considered in this work due to the limited accessibility of data (Palle et al., 2022). It can be clearly found that, for carbonaceous materials, of which the derivation of CO_2 capture performance from theoretical calculation is relatively difficult due to the structural complexity of activated carbons, the high-throughput screening on their CO_2 selectivity is unpractical at the current stage. This limitation urges the further development of available database that homogeneously describes the structural details of activated carbons in the future.

Polymers. Polymer-based membranes have been widely used in the selective separations of mixed gases like N_2/O_2 (Himma et al., 2019), N_2/H_2 (Ockwig and Nenoff 2007), CO_2/N_2 (Liu et al., 2016), and CO_2/CH_4 (Liu et al., 2018). Generally, permeability and selectivity are two critical criteria that determines the CO_2 separation performances of membranes, whereas these two criteria go against each other under real-world conditions, that is, higher the permeability is, generally lower the selectivity is achieved, and *vice versa*. However, it should be noted that, although these two parameters negatively correlate, and a 'Robeson plot' can be drawn based on this correlation, the upper limit of this plot continuously evolves with the dedications of scientists. The primary purpose of the involvement of ML-based studies in this area is further optimizing the upper limit of such 'Robeson plot'. It requires to screen and test the CO_2 separation performances of a large amount of polymer membranes, which significantly challenges the time-consuming experimental pathways.

How to digitalize the features of polymers, which contains complex ligands that may interact with each other in a twisted manner, is a critical challenge facing the application of ML in relevant fields. In 2020, Barnett et al. for the first time addressed

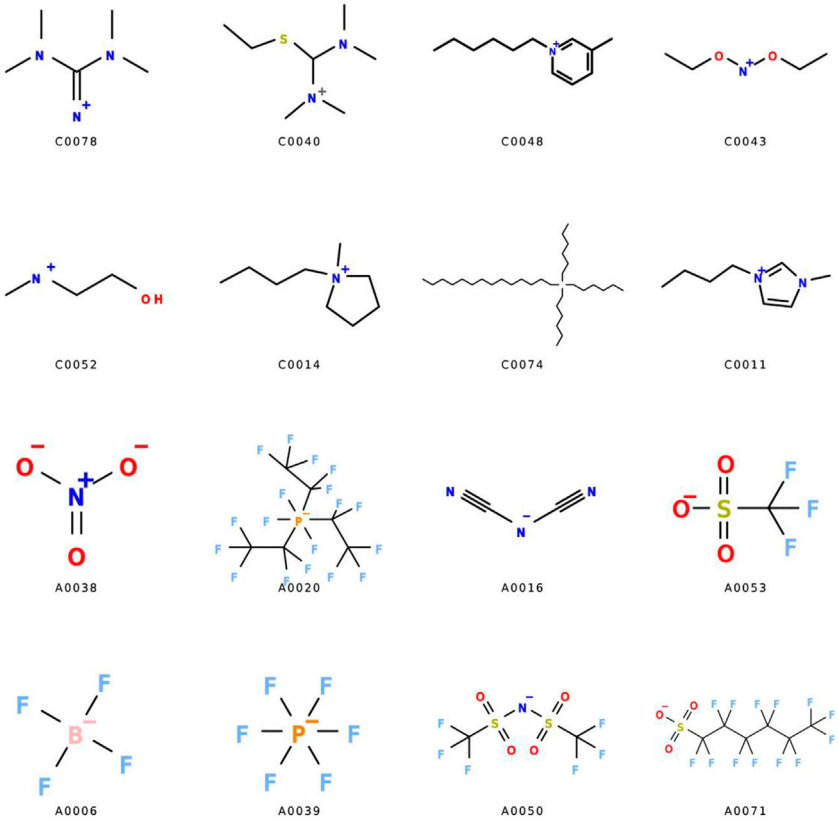


FIGURE 10
Prominent cations (prefixed with "C") and anions (prefixed with "A") found in the dataset (Venkatraman and Alsberg, 2017).

this issue by creating fingerprints for polymers based on topological methods (Barnett et al., 2020) (as shown in Figure 7). Specifically, the authors transformed each polymer into a binary fingerprint using the Daylight-like fingerprinting algorithm as implemented in RDKit. This topological-based approach analyzes the various fragments of a molecule containing a certain number of bonds and then hashes each fragment to produce a binary fingerprint that computationally represents the molecule. After a polymer's repeat unit was read into memory *via* a molfile, it was broken down into fragments containing between 1 and 7 units (represented for n = 1 to n = 4 in Figure 7), and the structure was hashed into a fingerprint with 2048 bits of information to encode all of the possible connectivity pathways of the monomer. This process is repeated for each group in the molecule to generate the full fingerprint. Each bit was treated as a single feature in our model, which allows us to study the effects of various functional groups and their linkages on gas transport. Each monomer was connected to at least nine other identical repeat units to properly account for longer paths along the polymer backbone. This fingerprinting technique is the simplest representation of the polymer chemistry and structure that is sufficient to capture trends observed in the experimental data.

Based on this novel method, the simulation results showed that two polymers, that is, poly [(1,3-dioxoisoindoline-2,5-diyl) sulfonyl (1,3-dioxoisoindoline-5,2-diyl)-1,4-phenyleneoxy-1,4-phenylene] (ID: P432092) and poly [(1,3-dioxoisoindoline-2,5-diyl) sulfonyl (1,3-dioxoisoindoline-5,2-diyl)-1,4-phenylenemethylene-1,4-phenylene] (ID: P432095) lied well above the upper limit of the 'Robeson plot' for CO_2/CH_4 separation (as shown in Figure 8). Both of these polymers are polyimides containing sulfone groups. Besides, P432092 contains an aromatic ether linkage, and each of these groups is highlighted during the analysis of the ML data as being related to high CO_2/CH_4 selectivity. In addition to this revolutionary study, another work also explored the permeability of different gas components through polymer membranes (Yuan Q. et al., 2021), and identified that the permeability followed the order $O_2 > CO_2 > N_2 > CH_4 > He$. Two outperforming polymer membranes locating above the Robeson upper limit 2008 were selected out, namely KAUST-PI-1 and PIM-1, for the separation of CO_2 and CH_4.

Zeolites. Zeolites refer to a group of porous materials with the general formula of $Mn^{+1/n}$ $(AlO_2)^-(SiO_2)_x{\cdot}yH_2O$, where $Mn^{+1/n}$ is either a metal ion or H^+. Considering the porous and functionalized nature of zeolites, they are widely used as commercial adsorbents for gaseous pollutant removal from

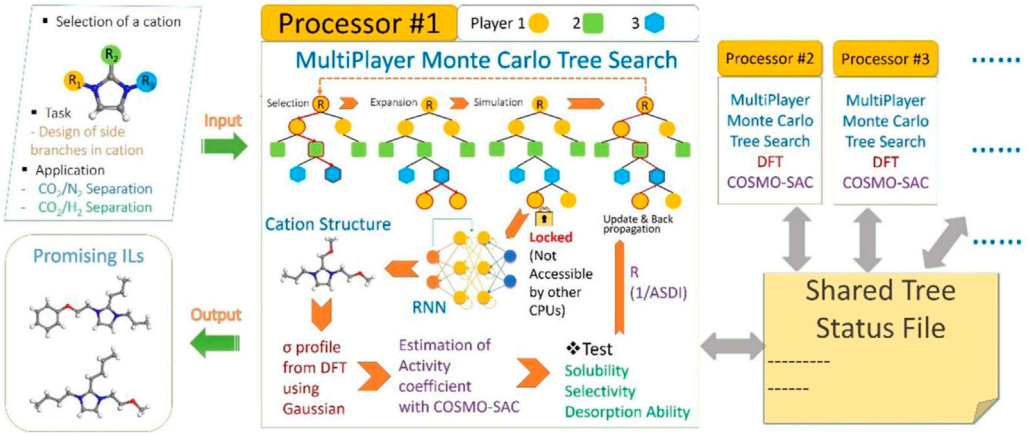


FIGURE 11
A schematic of our algorithm to design an application-specific ionic liquid (Zhang et al., 2021).

industrial flue gas (Ding and Yazaydin 2013; Sun et al., 2014; Bakhtyari et al., 2020; Ma et al., 2021). Several models including the Hybrid-ANFIS, PSO-ANFIS, and LSSVM had been proposed for the prediction of the CO_2 adsorption on various zeolites (Raji et al., 2022). The accuracy of the models was assessed based on calculating the MSE AARD, R^2, and STD. According to the results, it is shown that the all models are reliable and precise for estimating the CO_2 adsorption on various zeolites and applicable methods for the design and analysis of the CO_2 adsorption processes. It can be concluded from Figure 9 that pressure increment has a higher effect on the CO_2 adsorption performance than temperature. In Zeolite 5A, the effect of temperature was more obvious than other zeolites. For zeolite T type and ssz-13 in the temperature around 330 K, there can be seen an optimal point for CO_2 adsorption.

Absorbents

***Ionic liquids* (*IL*).** IL generally refers to a group of subset examples of molten salts fully comprised of abundant ions (anions and cations) with melting point below 100 °C (Lei et al., 2017; Zhang et al., 2021a; Zhang et al., 2021). Since the last decade when IL was found to be a promising absorbent for CO_2 capture (Blanchard et al., 1999), this group of nonvolatile and designable materials has been extensively explored for its functionalized role in related fields (Zeng et al., 2017). Purposefully and pertinently engineering the functional ligands in IL is the key challenge for the further improvement of CO_2 selectivity over other gas components and the applicability of IL-based CO_2 technologies. The intrinsic complexity of the synthetical and processing optimization makes ML an emerging and effective method to such a sophisticated end. The ways of data collection are categorized into two types, that is, collecting from previous studies and calculating based on theoretical methods. The former one merits for its precision in performing data analysis and processing, while the later one may contain a wider range of material variety for CO_2 capture.

In 2017, ML was for the first time used as a tool to investigate the CO_2 capture by ILs (Venkatraman and Alsberg, 2017), and the performances of different ILs were collected based on experimentally determined results (Lei et al., 2014). 185 ionic liquids (68 cations, 65 anions) comprised of 10,848 solubility measurements, which is widely inclusive, across different temperatures and pressures were used as the fundamental database for the model training and testing (Figure 10 showed prominent cations (prefixed with "C") and anions (prefixed with "A") found in the dataset). Both physical and chemical features, including the HOMO/LUMO energies, polarizabilities, superdelocalizabilities, charge partial surface areas (CPSA), and various geometrical indices as derived from semi-empirical MOPAC, were considered. The main goal of this work was examining the accuracy of different ML algorithms in fitting the CO_2 capture capabilities of ILs, and found that random forest was more suitable than decision tree and partial least squares regression in this case, probably attributed to the adaptability of random forest in learning datasets with considerable diversity and deviation. However, the R^2 as obtained equaling to 0.71 was still far from satisfactory due to such intrinsic complexity. A limited batch of ILs containing several designated functional groups was hence studied, aiming to attain more precise results within a specific IL scope (Mesbah et al., 2018; Daryayehsalameh et al., 2021). It was identified that, when only [Bmim][BF_4] ILs was considered, a NN-based ML model exhibited a much higher accuracy with R^2 equaling to

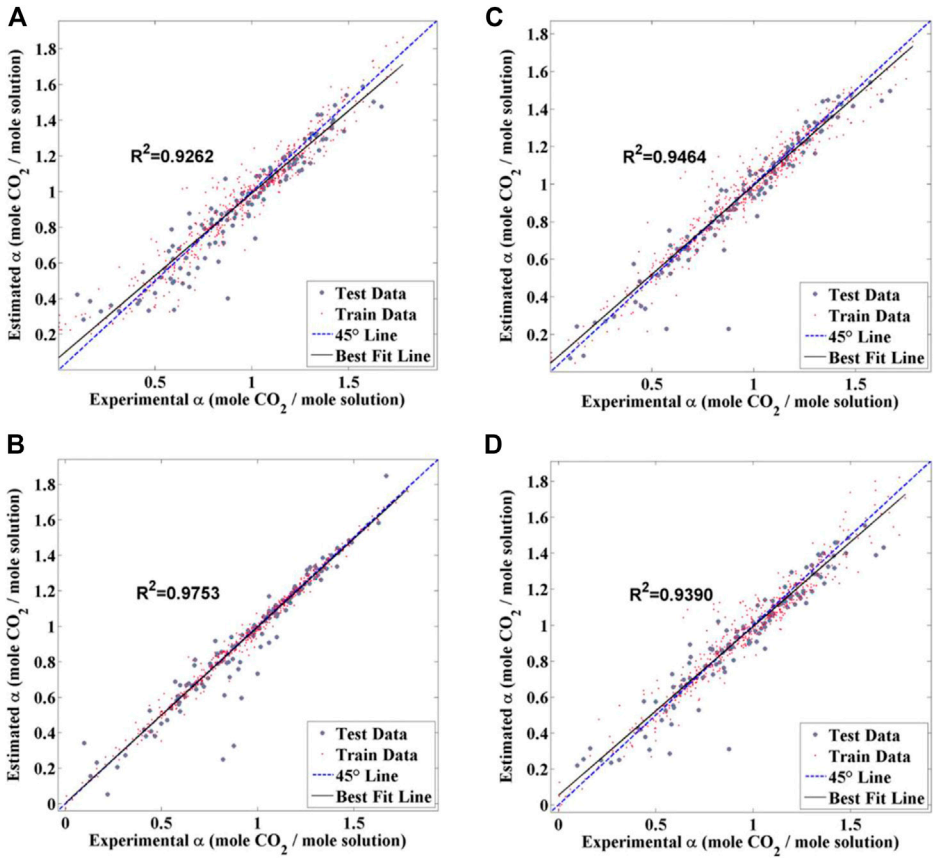


FIGURE 12
Regression plot for the absorption of CO_2 prognostication by **(A)** LSSVM, **(B)** RBF-NN, **(C)** PSO-ANFIS, and **(D)** ANFIS (Dashti et al., 2021a).

0.99 and 0.98 for the training and testing sets. The effects of pressure and temperature on the CO_2 capture performance of [Bmim][BF_4] ILs were predicted, indicating that a relatively high pressure and low temperature might be beneficial for CO_2 capture by [Bmim][BF_4] ILs. Besides, by using a relative sophisticated multi-layer NN-based model with group contribution (GC) methods, a satisfactory precision was also obtained for a wider scope of experimentally collected ILs with more than 10,000 data points (Song et al., 2020).

While extensive ML-guided studies have been conducted to study the laws of CO_2 solubility in ILs, there are still two critical issues remaining to be well-addressed, that is, 1) the predicament between the scale of IL database and the prediction accuracy due to the influence of diversified variables, and 2) the insufficient understanding of the selectivity of CO_2 over other gas components because of the limited amounts of relevant experimental results. To obtain an improved data homogeneity, the theoretically derived mass-based Absorption-Selectivity-Desorption index (ASDI) was adopted to characterize the selectivity of approximately 1000 IL systems towards CO_2/N_2 separation (Wang K et al., 2021). Cyano-based ILs were found to be excellent solvents for separating CO_2 and N_2, and Aspen Plus [EMIM][TCM] was selected as best IL, the process of which led to 12.9% savings on total annualized cost (TAC) compared to that of [EMIM][Tf_2N]. Following this effective method, a subsequent study extended the database of screened ILs to more than 400,000 by adopting the Simplified Molecular Input Line Entry System (SMILES) that sequences strings of symbols in ILs based on their graph theory (Zhang et al., 2021) (a brief illustration on the technical roadmap is shown in Figure 11). The ILs with sequencing number of CCCc1n (CCOc2ccccc2)cc [n +]1CCOC and CCCc1n (CCC)cc [n +]1CCOc1ccccc1 were found to exhibit superior performances towards the CO_2 separation from H_2 or N_2. However, as the authors did not consider whether the involved computationally derived structures can be successfully synthesized *via* experiments, further validation on the feasibility and applicability of these ILs needs to be conducted in the future.

To leverage both the structural motif of MOFs and the absorption ability of ILs, the CO_2 capture performances of IL-MOF composites were also scrutinized based on ML models

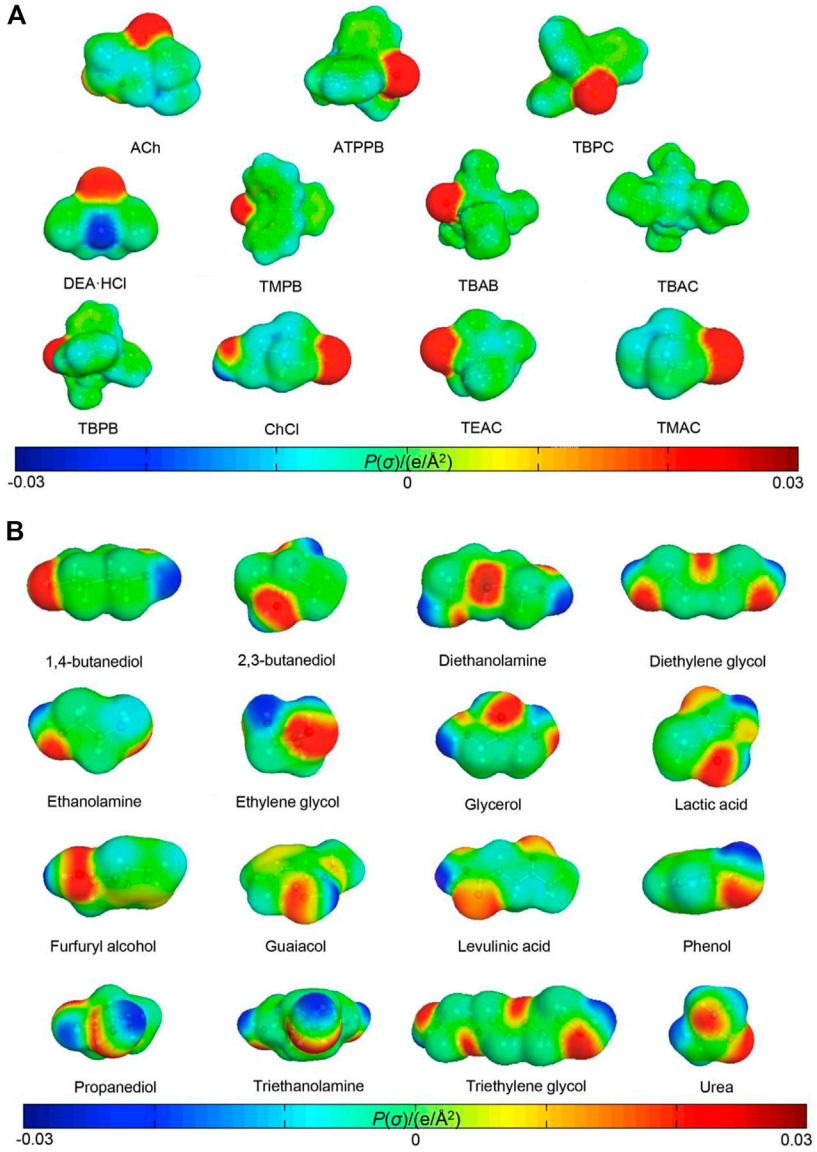


FIGURE 13
Optimized **(A)** HBA and **(B)** HBD structures with COSMO surfaces (Wang J et al., 2021).

(Zhang Z. et al., 2022). The configurational-bias Monte Carlo (CBMC) method was adopted to insert 1-aminopropyl imidazolium bis(trifluoromethylsulfonyl) imine ([NH_2-Pmim][Tf_2N]) into different MOFs. GCMC was used to calculate the adsorption capacity and CO_2 selectivity of IL-MOF composites, and the RF algorithm was taken to perform the ML process. It was identified that the accessible volume (AV), the density (ρ), and free volume (V_{free}) are three major influential factors affecting the CO_2/N_2 selectivity of IL-MOF composites. Structure-performance relationship revealed that IL-MOF with optimal AV (0.176–0.444 $cm^3\ g^{-1}$), ρ (1.295–2.046 $g{\cdot}cm^{-3}$), and V_{free} (1724–4785 $Å^3$) result in decent CO_2/N_2 selectivity. [NH_2-Pmim][Tf_2N]@ZIF-67, an IL-MOF composite exhibiting moderate CO_2 separation performance, was synthesized to successfully verify the accuracy of the ML simulation. However, it should be noted that, in this study, the authors primarily investigated how the change of MOF characteristics influenced the CO_2 separation performances of IL-MOF composites, while the features of ILs were skipped. Further scrutinization on the synergetic effects between ILs and MOFs are of great importance to make the performance prediction more practical and precise.

Amine-based absorbents. Amine-based materials have been widely commercialized for CO_2 capture from large-scale

industrial processes, MEA, piperazine (PZ), and N-methyldiethanolamine (MDEA) are the most studied absorbents in previous works (Dutcher et al., 2015; Yamada 2021). The mechanism of amine-based CO_2 capture technologies generally involves the reaction between amine and CO_2 to form carbamate anion ($NCOO^-$) and protonated amine (BH^+). The predominant merit of amine-based CO_2 capture technologies is its reversibility, that is, the feasible regeneration of spent absorbents *via* relatively facile and cost-effective methods, which significantly reduces the operation cost and makes the commercialization preferred. Due to the lack of applicable computational tools to obtain the absorption capacities of amine-based materials, previous studies all relied on experimental results to conduct ML studies in this field. Under this circumstance, the complex effects of external influential factors may become a major obstacle that impedes the derivation of a highly consistent conclusion. Thus, ML based methods, as an effective method to generalize parameters, began to assist practitioners in designing the next-generation amine absorbents, which may be applicable for highly selective CO_2 capture.

As a widely adopted amine-based absorbents, PZ was taken as the first example in ML screening and prediction for its CO_2 capture performance (Yarveicy et al., 2018). More than 1000 data points were collected from previous studies, and the reaction temperature, CO_2 partial pressure, and the concentration of PZ were featured as descriptors to explore the influence of external factors on the CO_2 separation performance of *p*Z. Four different algorithms including NN, adaptive neuro-fuzzy inference system (ANFIS), SVM, and DT were tested for their suitability and accuracy in this case. It was found that the DT-based algorithm exhibited the highest accuracy with the R^2 reaching ~0.99. A conclusion was drawn that CO_2 partial pressure had the predominant impacts on the CO_2 absorption performance of PZ, followed by the concentration of PZ and the reaction temperature. Under the optimal reaction condition, that is, reaction temperature, the concentration of PZ, and CO_2 partial pressure equaled to 313.15 K, 1.913 mol L^{-1}, and 7.51 kPa, the absorption capacity of PZ towards CO_2 was 0.86 mol CO_2 per mol *p*Z. Besides, the influences of reaction temperature, CO_2 partial pressure, and the concentration of amine on the CO_2 absorption performance of MEA, diethanolamine (DEA), and triethanolamine (TEA) were also scrutinized (Ghiasi et al., 2019). It was surprisingly found that for different amines, the dominant experimental condition changed. Specifically, for MEA and TEA, the importance of different experimental conditions followed the order reaction temperature > partial pressure > the concentration of amines, while for DEA, the order changed to partial pressure > reaction temperature > the concentration of amines. Although errors may exist due to the insufficiency of experimental data, this work also gives valuable implications on the diversity of amine design.

Subsequent studies further extended the variety of descriptors and amines to provide more generalized guidance for absorbent optimization. In addition to reaction temperature, the pressure of flue gas, the flow rate, the pressure of re-boiler, reboiler duty, and condenser duty were also considered to further approximate the practical scenarios (Shalaby et al., 2021). An optimized operation condition was obtained to be flow rate = 4.01 mol s^{-1}, temperature = 319.7 K, the pressure of flue gas = 103.5 kPa, reboiler pressure = 160.0 kPa, reboiler duty = 153,600 W, and condenser duty = 8600 W. It could be found that the optimal reaction temperature as obtained under a relatively complex condition did not deviate from that obtained under simple conditions. Besides, the CO_2 capture performance of a novel group of amine-based absorbents, that is, amino acid salt (AAs), were also recently explored by ML-based methods (Pakzad et al., 2020; Dashti et al., 2021a; Mehrabi et al., 2022). In these studies, the intrinsic features of amines, covering the molecular weight of AAs, hydrogen bond donor count, hydrogen bond acceptor count, rotatable bond count, and heavy atom count, were for the first time co-considered with the external influential factors. Different algorithms including SVM, NN, ANFIS, and particle swarm optimization-ANFIS (PSO-ANFIS) were adopted to perform the simulation, among which the NN-based one exhibited the highest accuracy (as shown in Figure 12). The rotatable bond count and the molecular weight of AAs were identified to be the predominant factors influencing the CO_2 capture performance of AAs.

Deep eutectic solvent (***DES***). DES is a new generation of IL analogues sharing similar physicochemical properties as IL, such as negligible vapor pressure, high chemical/thermal stability and easily tunable character. Compared to ILs, DESs offer two advantages: 1) DESs can be prepared easily by mixing a hydrogen bond acceptor (HBA) with a hydrogen bond donor (HBD), avoiding complex synthesis and purification steps for ILs; 2) A large number of cheap and renewable compounds can act as the HBA (e.g., ammonium and phosphonium salts) or HBD (e.g., organic alcohols and acids), making DESs more affordable and sustainable over ILs. Using DES for CO_2 capture was extensively investigated in recent years, and ML-based methods were adopted to screen different DESs for their CO_2 absorption performances (Dashti et al., 2021b; Wang K et al., 2021).

A typical example to design DESs CO_2 absorbents with the assistance of ML-based methods was the application of a random forest derived ML model for performance description (Wang J et al., 2021). Before conducting ML studies, the structures of HBA and HBD of EDSs were first optimized using Gaussian software package (as shown in Figure 13). The red part and the blue part represent positive COSMO charge density and negative charge distribution, respectively. In order to generate the desired COSMO-RS-derived descriptors, the obtained COSMO files are directly imported into the COSMOthermX software to output the σ-profiles of HBAs and HBDs. The qualitative analysis from multiple linear regression shows that the variables, including the descriptors of HBAs and HBDs, molar

ratio of HBA to HBD as well as the temperature and pressure, are efficient input parameters for predicting CO_2 solubility in DESs. The importance of the involved variables in the QSPR model is ranked as pressure > HBA type > HBD type > HBA:HBD molar ratio > temperature.

Outlooks and conclusions

In the past 5 years, due to the rapid development of artificial intelligent and the explosion of material database, ML has stepped into the CO_2 separation area as an effective and efficient tool for ab-/adsorbent screening and design. Various ML algorithms including but not limited to MLR, RF, NN, DT, and SVM demonstrated their powers in this process where time-consuming and costly experiments were skipped. The CO_2 capture performances of several types of materials were simulated and scrutinized by ML-based methods. Novel materials that might serve the future benefits of carbon capture and sustainable energy conversion were proposed, parts of which proceeded far ahead of the current synthetical techniques. These achievements fully reflect the huge potentials of ML in improving CO_2 capture technologies, while the following issues may be the primary concerns to be well-addressed in the future to uncover these potentials.

The first issue is the establishment of consistent and integrated databases that make the influence of microcosmic descriptors more explorable. In previous studies, different scientists generally conducted experiments under varied conditions, and such variety made the effect of the intrinsic properties of materials hard to be identified. In this case, the explorers must firstly take the experimental conditions into consideration to train a reasonable model. However, the inclusion of external factors only contributes marginally to the rationally design of materials. Besides, it is noted that the criteria used to judge the CO_2 capture performance was different in different works, and the typical criteria used included the CO_2 capacity, the selectivity of CO_2 over other gas components, and the CO_2 removal efficiency. In a specific work, there were only one to two criteria being adopted, which further impedes the generation of integrated data in ML studies. Thus, it is suggested that a consistent experimental condition will be adopted for a same type of materials, and an integrated testing on its CO_2 capture performances involving diverse criteria, especially the CO_2 selectivity, is highly preferred.

The second issue is the development of effective methods to digitalize the structural properties of materials. Although the CO_2 adsorption over a wide variety of materials has been investigated, it is found that the descriptors used in most works were primarily the textural and compositional properties of materials. A sophisticated method to digitalize and visualize the complex interactions among atoms and ligands in the materials remains yet to be well-developed, while such inherent properties may play predominant roles in CO_2 capture, especially in cases where CO_2 is chemisorbed by sorbents like solid-state metal salts, which have hardly been investigated by ML-based pathways due to the lack of digitalized methods to feature their properties. To this end, topological method may be an extremely useful tool. However, due to the interdisciplinary nature to achieve the digitalization of such complex features, it was rarely applied in previous studies. Overcoming this critical challenge requires the participation and dedication of more interdisciplinary talents with both computer science and material science backgrounds in the future.

The third issue is the validation of the accuracy of ML-derived results. Despite the effectiveness ML displaying in designing CO_2 capture agents, it must be admitted that experimental verifications had rarely been adopted to justify the performances of these agents. The evidence of the accuracy of ML-based studies stuck in a non-rigorous cycle where the CO_2 performance was obtained from calculation, and a similar calculation process was conducted to test its validation. While self-consistent results could be generated on this basis, they may be far from the real outcomes obtained under practical scenarios. This is why this review urges the attention to the selectivity of CO_2 because no practical condition can ignore the influence of interfering gas components. Besides, this challenge also identifies the importance to conduct experimental verification on the ML-derived results. Otherwise, the application of ML in CO_2 will only be a costly activity rather than a beneficial pathway towards the mitigation of climate change in the future.

Author contributions

ZY organized the analysis and wrote the manuscript, BC collected the data and revised the manuscript, HC collected the data, and HL conceived and supervised the research.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

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