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Review

Intelligent prediction of ionic liquids and deep eutectic solvents by machine learning

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ABSTRACT

Ionic liquids (ILs) and deep eutectic solvents (DESs) as green solvents have attracted dramatic attention recently due to their highly tunable properties. However, traditional experimental screening methods are inefficient and resource-intensive. The article provides a comprehensive overview of various ML algorithms, including artificial neural network (ANN), support vector machine (SVM), random forest (RF), and gradient boosting trees (GBT), *etc.*, which have demonstrated exceptional performance in handling complex and high-dimensional data. Furthermore, the integration of ML with quantum chemical calculations and conductor-like screening model-real solvent (COSMO-RS) has significantly enhanced predictive accuracy, enabling the rapid screening and design of novel solvents. Besides, recent ML applications in the prediction and design of ILs and DESs focused on solubility, melting point, electrical conductivity, and other physicochemical properties become more and more. This paper emphasizes the potential of ML in solvent design, overviewing an efficient approach to accelerate the development of sustainable and high-performance materials, providing guidance for their widespread application in a variety of industrial processes.

1. Introduction

Ionic liquids (ILs) are a kind of unique material which are liquid state at or near normal temperature [1]. They are generally composed of organic cations and organic or inorganic anions through ionic bond. In 1992, a series of imidazolyl ILs that could remain stable of physicochemical property after exposure to air and water were reported by Wilkes *et al.* [2]. Subsequently, the ILs obtained extensive research and close attentions due to their advantages, such as low volatility, high conductivity, high thermal conductivity, high stability, wide electrochemical window, and so on [3–8]. With the specific features made ILs applicable in various fields of chemical engineering, including the chemical separation, green solvent, catalysis, chemical reactive synthesis, biochemistry, electrochemistry, *etc.* [9–13]. In addition, deep eutectic solvents (DESs) have many uniform characteristics and properties as ILs, which is first named by Abbott *et al.* in 2004 [14]. DESs are composed of hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) through hydrogen bond. Similarly, DESs also have many advantages, however, the structure and properties of ILs is determined by cationic and anionic ions, while the DESs' is determined by hydrogen bond between HBD and HBA. Whereas, one of the unique characteristics for both ILs and DESs is the tunable and designability [15–17]. That is to say, a large number of ILs or DESs could be obtained by combining different cations and anions or different HBD and HBA, especially for ILs, it could be as much as 10^{18} theoretically [18,19]. This means that it will be very difficult to acquire suitable ILs or DESs for corresponding applications by traditional experiments. Therefore, seeking effective and rapid methods to replace extensive experiments to screen ILs or DESs became the research focus.

These years, some common prediction methods have been developed to assist to screen ILs or DESs, such as equation of state (EoS) [20,21], group contribution (GC) [22–24], conductor-like screening model (COSMO) [25–27], molecular dynamics simulation [28,29], and so on. Recently, with the rapid development of

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computer technology, artificial intelligence (AI) has profoundly changed the current research paradigm. Compared with the traditional prediction methods like above-mentioned, AI can provide faster and more accurate data prediction and processing, and has become an essential tool in scientific research. Machine learning (ML) is the core of AI, which is a powerful tool for finding rules in high-dimensional data, and has applied in the fields of chemical engineering, advanced material, medicine, and so on [30–33]. Generally, we can take the ML model as a tool and construct quantitative structure-property relationship (QSPR). QSPR is a method that relates physical or chemical properties with molecular structure based on molecular descriptors, and effectively predicts the properties of substances by building a relationship model between structure and property. Compared with other methods, it has the advantage that only chemical structure information is required, and it has nothing to do with any experimental properties [34–36]. Combined ML model and QSPR, through learning of a large amount of known experimental data (input descriptor) and identifying the potential links between data and results (output descriptor) without relevant physical, chemical or biological processes, has the potential for significant cost savings and efficiency improving, especially for the huge amount of ILs and DESs.

In fact, the construction of QSPR model combined with ML models has been widely used in the prediction and screening the properties of ILs and DESs, and has obtained some research achievements. Here, we will focus on the application of ML models on ILs or DESs, and conclude recent progress of the relevant properties prediction. Firstly, we will introduce some common ML models for ILs or DESs property prediction, then we will conclude the progress of each property prediction by ML models, in order to provide reference for correct choose of ML models, as well as the correct screening and structural design of ILs and DESs.

2. Machine Learning Algorithm

2.1. Models

As a method that can provide more efficient and accurate data prediction and processing, AI has become an essential tool in scientific research. Similarly, in the fields of prediction and effective screening of various properties of ILs or DESs, AI-based ML methods are also widely used and show excellent performance. There are various kinds of ML methods, which can be generally divided into supervised learning, unsupervised learning, semi-supervised learning, *etc*. The input data of supervised learning is labeled samples, the input data and output data are provided at the same time, and the model is generated by training the labeled input data. Unsupervised learning does not provide labeled samples, but it can find hidden associations and rules from given data by the model itself. Whereas semi-supervised learning is based on two types of data, labeled samples and unlabeled samples. In the prediction of ILs or DESs properties, supervised learning method is often adopted, that is, input variables and output variables are provided at the same time, and a model between input variables and output variables is built based on existing big database.

From the study of Yusuf *et al.* [37], ML models used to predict the physicochemical properties of ILs were divided into two categories, namely traditional model and mixed model. Traditional models include least square support vector machine (LSSVM), artificial neural network (ANN), adaptive neural fuzzy inference system (ANFIS), *etc*. The mixed model includes random forest (RF), gradient boosting regression (GBR), data processing group method, and so on. In general, the different models will be selected for different property prediction.

For various prediction models, we can further divide them into several categories based on model structure, which are linear models, neural networks, tree models, kernel methods, probabilistic models, etc. In the following, we will introduce them in detail.

2.1.1. Linear models

Multiple linear regression (MLR) is one of the simplest and most common ML methods, which is used to establish the corresponding relationship model between an output variable and multiple input variables. The formula can be described as follows,

$$y = a_1x_1 \pm a_2x_2 \pm a_3x_3 \pm \cdots \pm a_nx_n \pm a_0$$

in which, y is the output variable, x_1-x_n are the input variables, and a_1-a_n are the coefficients. When applied to the construction of structure-property prediction model, it is generally recognized that the symbol before the coefficient represents the qualitative influence law of input variables on output variables, that is, the plus sign represents the positive correlation between input variables and output variable, and the minus sign is the opposite, representing the negative correlation between input variables and output variable. But in most complex processes, MLR can't provide accurate prediction results. Therefore, it is necessary to find more accurate and comprehensive ML models.

2.1.2. Neural networks

Neural network (NN) is a powerful model that mimics the structure and function of biological nerve cells. It can solve the problems of both regression and classification by forming hierarchical and connectivity relationships. Amongst, ANN is the foundation and typical representative of NN models and has been applied in many prediction research, including various physical-chemical properties prediction of ILs and DESs due to its rapidity and accuracy [38–40]. Generally, the ANN model has several layers, including input layer, one or more hidden layers and output layers, the schematic diagram is shown in Fig. 1(a).

The convolutional neural networks (CNN) which is also widely applied on the prediction in the fields of chemical engineering. It consists of convolution layer, pooling layer, and fully connected layer. The convolution operation is carried out by sliding on the data through the convolution kernel to automatically extract local features, and the pooling layer can reduce the data dimension and retain key features. Compared to ANN, the number of parameters and calculation amount of the CNN model are greatly reduced, and the training efficiency and generalization ability are improved.

Besides, there are other NN models like feedforward neural network (FNN), back propagation neural network (BPNN), radial basis function neural network (RBFNN), cascade-forward neural network (CFNN), hybrid neural networks (HNN), and so on.

2.1.3. Tree models

Tree models are a kind of model widely used in various fields of engineering. It takes into account the ability to solve both regression problems and classification problems [43–45]. For tree models, there are decision tree (DT), gradient boosting trees (GBT), RF, *etc*. RF and GBT are two typical tree models based on decision trees and both are powerful supervised learning algorithms. They are both ensemble models, but RF builds the trees in parallel, whereas the GBT builds the trees in series. The RF model builds the trees through a random way and it is a bagging ensemble model, that is to say, in which the sub-data set is sampled and then the sub-model is trained with a new training set. While the GBT builds the trees by a continuous way and is a boosting ensemble model which means each next tree tries to correct the error of the

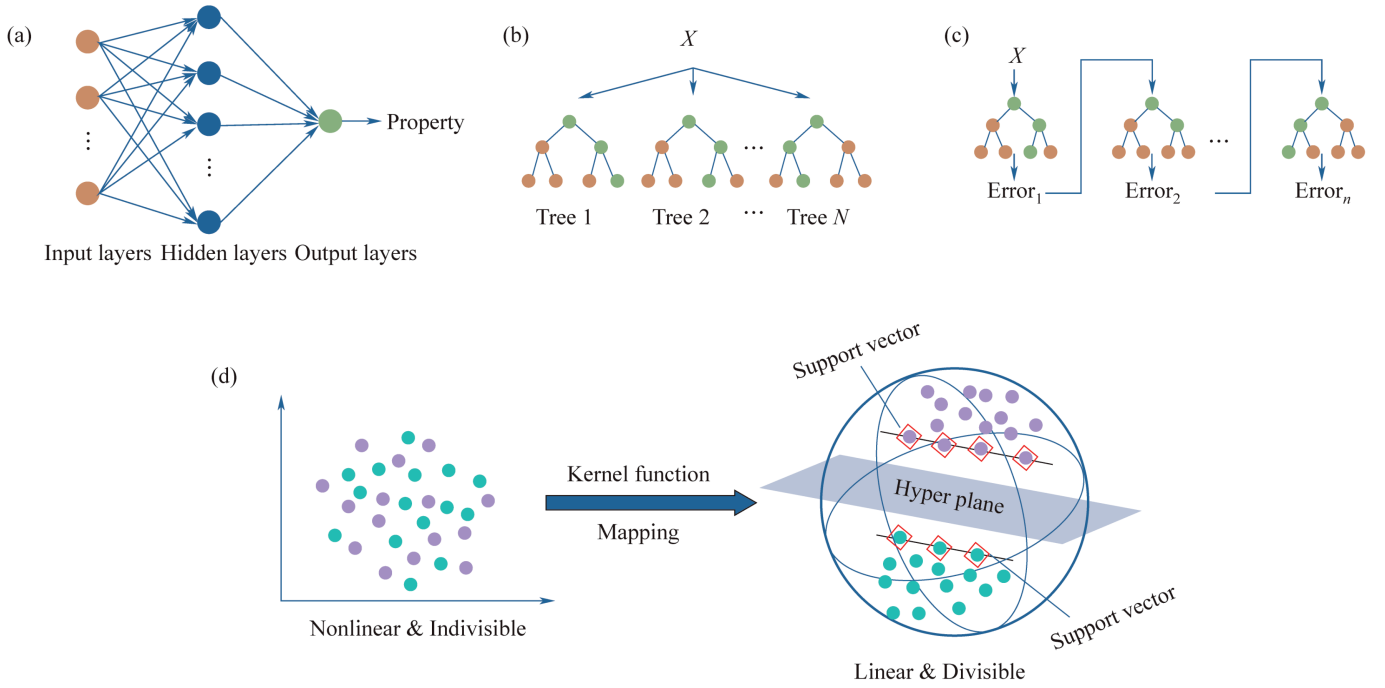

Fig. 1. Scheme diagrams of ML models: (a) ANN, (b) RF, (c) GBT, and (d) SVM. [41], copyright 2023, *Journal of Molecular Liquids*. [42], copyright 2024, *Chemical Engineering Science*.

previous one, the schematic diagrams for both RF and GBT are shown in Fig. 1(b) and (c).

Based on different ways of trees construction, RF and GBT have their unique advantages. The parallel structure of the RF model make it can greatly reduce the calculation time and load to get the benefit of efficiently handling large databases. Compared with RF, the series structure of the GBT model makes the calculation speed a bit slow, but it is more sensitive to parameter settings. Therefore, the RF model has stronger generalization ability, while the GBT model is more sensitive to outliers. But anyway, both RF and GBT models are widely used as prediction models for the properties prediction of ILs and DESs and show excellent prediction performance.

2.1.4. Kernel methods

The kernel function method is a powerful tool for dealing with high-dimensional data and non-linear problems. Its core idea is to map data from the original space to a high-dimensional feature space using a kernel function. In this high-dimensional space, the data that are non-linearly inseparable in the original space may become linearly separable. The kernel function can effectively compute the inner product of two data points in the high-dimensional feature space without explicitly calculating the coordinates of the data points in the high-dimensional space. Common kernel functions include the linear kernel, polynomial kernel, and radial basis function (RBF) kernel, among others.

Amongst, the support vector machine (SVM) model is one of the typical kernel function methods introduced by Vapnik [46,47]. It has been applied on widespread chemical engineering fields including structure–property relationship prediction, such as phase equilibrium, physical-chemical properties, toxic activity, *etc.* due to the simple structure and excellent prediction performance [47–50].

For the SVM model, it is based on Vapnik Chervonenkis (VC) dimension theory and the structural risk minimization principle. It can handle both classification and regression tasks. As described above, the kernel function is the link between non-linear groups and linear groups. We can find from Fig. 1(d), the disordered non-linear groups can be rearranged into linear and divisible groups through kernel function and corresponding the created boundary called hyper plane. As well as the rearrangement process from non-linear lower dimensional space to linear higher dimensional space is called mapping, and the following prediction task will be handled in the rearranged linear higher dimensional space.

2.1.5. Probabilistic models

Probabilistic models are a class of models that use probability distributions to describe data generation processes or make predictions, and are widely applied in the field of chemical engineering, including ILs and DESs properties or toxicological prediction. These models handle uncertainty through a probabilistic framework and use probability theory to describe random phenomena or uncertain events. Probabilistic models can be discrete or continuous, including generative models, discriminative models, Bayesian models, and non-parametric models, *etc.*

Take Bayesian models as an example, which are an important subclass of probabilistic models based on Bayes' theorem. Bayesian models combine prior probabilities and likelihood functions to compute posterior probabilities and can be applied to inference, prediction, and decision-making tasks. Their core strengths lie in handling uncertainty, incorporating prior knowledge, and supporting dynamic updates which allows models to naturally incorporate prior information when dealing with uncertainty and dynamically update inference results as new data. The application of Bayesian models in the field of ILs and DESs shows the powerful ability in dealing with complex systems and uncertain problems. By combining deep learning and ML techniques, Bayesian models can not only improve the accuracy of property prediction but also play an important role in fault diagnosis and optimal design of chemical processes. In the future, with the further development of Bayesian models, the application prospects will be more extensive.

2.2. Input descriptor

For the construction of machine learning models, the selection of input variables has an important impact on the reliability and accuracy of ML model prediction results. At present, there is no unified standard for the selection of input variables. Taking predicting gas solubility in ILs or DESs as an example, the input descriptors can be roughly divided into several categories. It mainly includes the thermodynamic properties (such as molecular weight, temperature, pressure, eccentricity factor, critical properties, *etc.*), types or numbers of atoms, functional groups, molecular fingerprints, quantum chemical descriptors, *etc.* [51–53]. For example, Barati-Harooni *et al.* [54] took temperature, pressure, molecular weight of IL, number of carbon atoms in cations, number of carbon atoms in anions, number of hydrogen atoms in anions, number of IL nitrogen atoms, number of IL sulfur atoms, number of IL oxygen atoms, number of IL fluorine atoms, number of IL chlorine atoms, and number of IL boron atoms as input variables. Then radial basis function neural network optimized by particle swarm optimization method (PSO-RBF), multilayer perceptron neural network (MLP-NN), least square support vector machine optimized by coupled simulated annealing (CSA-LSSVM), and adaptive neuro-fuzzy inference system trained by hybrid method (Hybrid-ANFIS) models were used to predict the solubility of CO_2 and H_2S in ILs, and it was found that the average absolute relative deviation (AARD) of the four models was less than 5%, which was better than that of the thermodynamic model. Morgan fingerprint is a method to generalize molecular characteristics by using molecular structure information. Jian *et al.* [51] generated 4096 Morgan molecular fingerprints through the RDKit program. With temperature and pressure as input variables, SVM, RF, extreme gradient boosting (XGBoost) and MLP models were used to predict the solubility of CO_2 in ILs. It was found that MLP has an excellent prediction effect. The quantum chemical descriptors can represent the structural characteristics of ILs. For example, Mehraein *et al.* [55] obtained the number of single bonds, average bonding information content, and solvation energy graph of different ILs as input variables after Gaussian optimization of IL structures. Genetic algorithm-multi linear regression (GA-MLR) and LSSVM models were applied to predict the solubility of CO_2 in ILs, and LSSVM was found to have better prediction performance. In short, with the deepening of the research, the used input descriptors have evolved from the initial simple physicochemical properties to complex descriptors, including the structure and internal characteristics. Optimization of input descriptors combined with other methods can greatly improve the accuracy and reliability of ML models' prediction of ILs or DESs properties. Recently, the decoder such as simplified molecular input line entry system (SMILES) has always been used for the transformation of chemical structures into SMILES strings and then takes the SMILES strings as input descriptors for highly efficient and accurate computer processing and analysis.

3. Application of Machine Learning on Prediction of Ionic Liquids

As mentioned above, we have learned that the ML methods are diverse and have become an important tool in scientific research. Meanwhile, the quantity of ILs is huge, and screening only through experiments will cost a lot of manpower and material resources. Therefore, building the relationship of composition-structure-function-property based on methods such as computer and theoretical simulation will be the future development trend. In this section, we will mainly summarize and describe the prediction of solubility, toxicity, physicochemical properties, as well as the design and screening of ILs.

3.1. Solubility prediction

ILs, as a kind of green solvent, exhibit excellent solubility for many gases. Research on the solubility of gases in ILs is of great significance for studying intermolecular interactions, phase equilibrium, pollutant gas absorption, greenhouse effect emission reduction, and other aspects. With the continuous progress of various technologies, many methods have been used in the prediction of gases solubility in ILs. Amongst, ML prediction models have gotten more and more attention with the rapid development of computer technology.

Recently, in the requirement of tackling global climate change and reducing greenhouse gas emissions, the implementation of carbon dioxide (CO_2) capture technology is particularly critical and urgent. It is expected to predict CO_2 solubility in ILs by ML methods quickly, efficiently and accurately, as well as screening suitable ILs for CO_2 adsorption. In the manuscripts, a variety of ML models and input descriptors were used by researchers. Jian *et al.* [51] developed two kinds of ML models, which are fingerprint-based ML models and graph neural network (GNN) to predict the CO_2 solubility in ILs. Especially the GNN models can handle tasks in both the feature extraction stage and the model prediction stage, demonstrating the effectiveness of the GNN model in learning from graphical data. The way for the connection of the matrix and GNN models prediction process for CO_2 solubility is shown in Fig. 2. Meanwhile, in this research, the authors also provided the functional groups importance ranking by the substructure-based explanation method, making the design of new ILs become possible. Further, Liu *et al.* [56] adopted other tools to obtain input descriptors. They used structure encoding (SE) and convolutional autoencoder (CAE) to transform and encode the molecular structure to molecular descriptors, then the models of RF, SVM, and MLP were constructed to predict the CO_2 solubility in ILs with the two input descriptors. All six models performed excellent prediction results, demonstrating that tools are useful for obtaining effective input descriptors. In addition to this, there was also some research to predict the selectivity of CO_2 with other gases, such as CO_2/N_2, CO_2/H_2, CO_2/CH_4, CO_2/C_2H_6, CO_2/C_2H_4, *etc.* [57,58].

In addition to CO_2, the solubility of many other gases in ILs has been predicted by building ML models, such as the H_2S solubility in ILs was predicted by LSSVM, deep belief network (DBN), XGBoost, Gaussian process regression (GPR), extreme gradient boosting (*i.e.*, XGBoost), RF, and SVM, *etc.* [59–62]; and N_2, N_2O, O_2 solubility in ILs was predicted by DBN, categorical boosting algorithm (CatBoost), extreme learning machine (ELM), extreme gradient boosting (XGB), two-layer feedforward neural network (TLFFNN), SVM, ANN, RF, GBR, DBN, multivariate adaptive regression splines (MARS), and extreme gradient boosting (XGB), *etc.* [41,42,63–65].

3.2. Toxicity prediction

In practical applications, the toxicity of ILs is a very important indicator, which is crucial for ensuring safety in industrial, environmental, and biomedical fields. ML provides the possibility for accurate and rapid prediction of the toxicity of ILs. Whereas, obtaining reliable toxicity data is fundamental to computer simulation studies. Currently, there are several databases related to ILs, but most of them cannot be used for toxicity prediction. For instance, PubChemand ChEMBL is large-scale chemical databases that allow querying relevant data through chemical names, CAS numbers, *etc.* [66]. However, these databases are not specifically designed for ILs. The UFT/Merk IL Bioeffects Database once

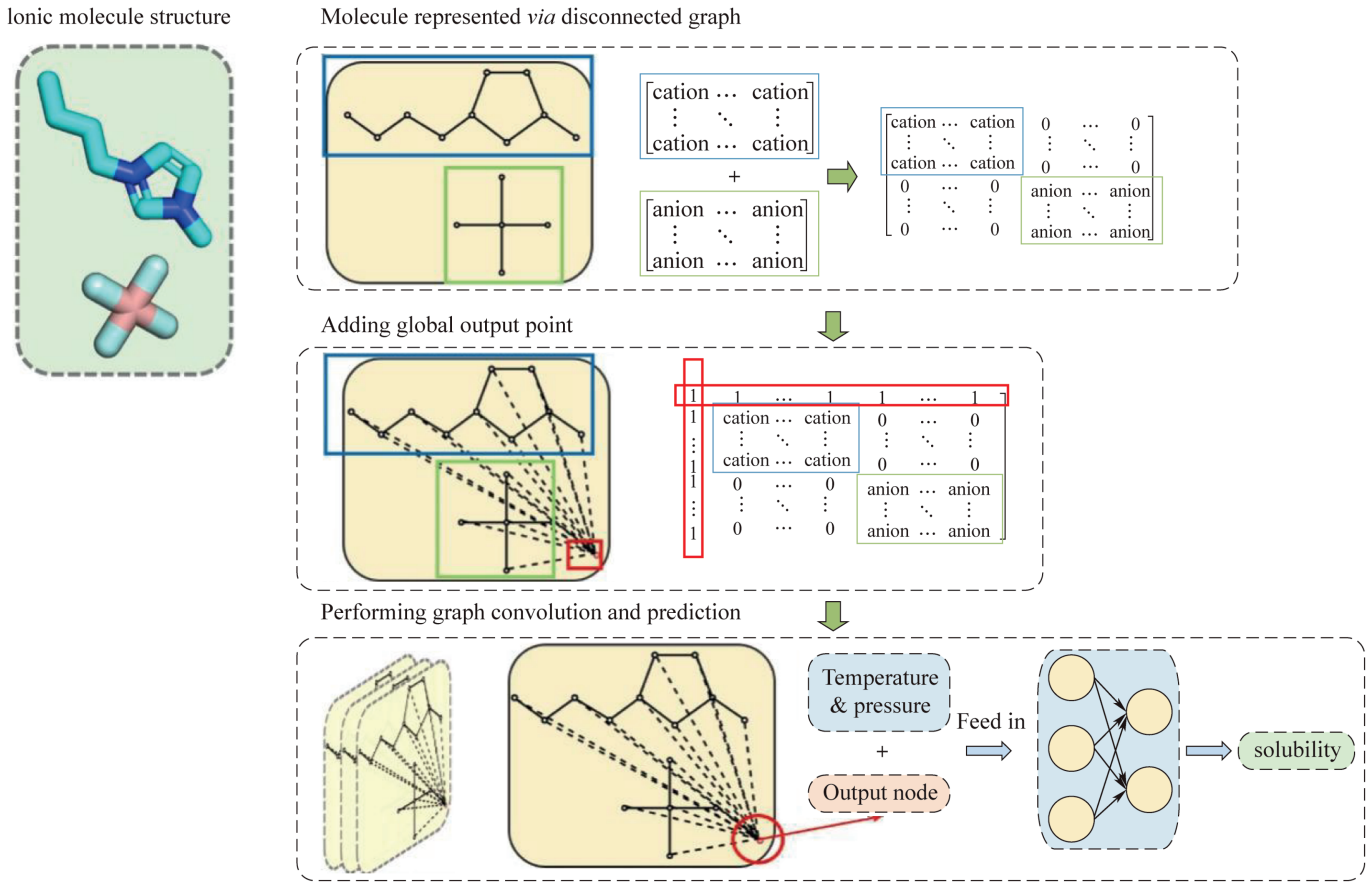

Fig. 2. GNN model prediction process for CO_2 solubility [51], copyright 2022, *ACS Sustainable Chemistry & Engineering*.

contained extensive data on the biological effects of ILs, but the website is no longer active. The International Union of Pure and Applied Chemistry has facilitated the establishment of the IL Database (IL Thermo), but which only collects thermophysical properties and mixture data of ILs. To fill the gap of lacking an IL toxicity database, researchers have proposed ILTox, a manually managed database specifically designed for toxicity assessment of ILs. This database integrates 6726 toxicity data entries for 1183 ILs, providing a wealth of data resources for studying IL toxicity. ML models built upon this database can analyze structure-toxicity relationships and screen 8 million virtual ILs, supporting the design of environmentally friendly ILs. Additionally, a data matrix recompiled by Alessio Paterno encompasses various biological toxicity data for 451 ILs, offering robust support for subsequent ML, deep learning, and molecular simulations in the field of IL toxicity research [67].

Recently, ML algorithms have been utilized to construct prediction models for efficiently and accurately assessing the toxicity of ILs. This method analyzes the relationship between the structural characteristics of ILs and their toxicity, aiding in the understanding of the toxicity mechanisms of ILs and providing theoretical support for the design and development of environmentally friendly ILs. Based on existing IL datasets, researchers have employed various ML and deep learning techniques to build predictive models for forecasting the potential toxicity of ILs. For example, in predicting the toxicity of ILs towards the leukemic rat cell line (IPC-81), toxicity data for 355 ILs were collected, and models were constructed using FNN and SVM algorithms [68], as shown in Fig. 3. After optimizing hyperparameters through five-fold cross-validation, the SVM model achieved determination coefficients (R^2) of 0.9289 and 0.9202 on the training and test sets, respectively, demonstrating good predictive performance. In predicting the toxicity of ILs towards Vibrio fischeri, RF and XGBoost models were utilized, with Bayesian optimization employed to adjust hyperparameters and five-fold cross-validation enhancing robustness. Results showed that the XGBoost model exhibited superior generalization ability with an R^2 of 0.957. Additionally, the SHapley Additive exPlanations (SHAP) analysis was applied, which can provide interpretability of the model decision-making process by fairly distributing the changes in the output to various features, and can be used to quantify the contribution of each feature to the prediction results of ML models. Through SHAP analysis, descriptors such as C2, C3, and C4 (C1-C5 represents descriptors produced by cations) were found to have significant impacts on both RF and XGBoost models, with increased cationic side chain length enhancing toxicity and ILs containing [NTf_2] anions exhibiting higher toxicity [69]. In predicting the inhibitory effect of ILs on acetylcholinesterase (AChE), RF and XGBoost algorithms were used to construct quantitative structure-activity relationship (QSAR) models, and 14 key molecular descriptors were screened. It was found that cations had a significant impact on AChE toxicity, with hydrophobic cations exhibiting more pronounced inhibition. The degree of branching, atomic weight, and partial charges of cations also influenced the inhibitory effect [70]. In terms of the toxicity of ILs to aquatic organisms, 5 ML methods were used to construct toxicity prediction models for D. magna, zebrafish, and R. subcapitata. It was discovered that cationic structure was a key factor

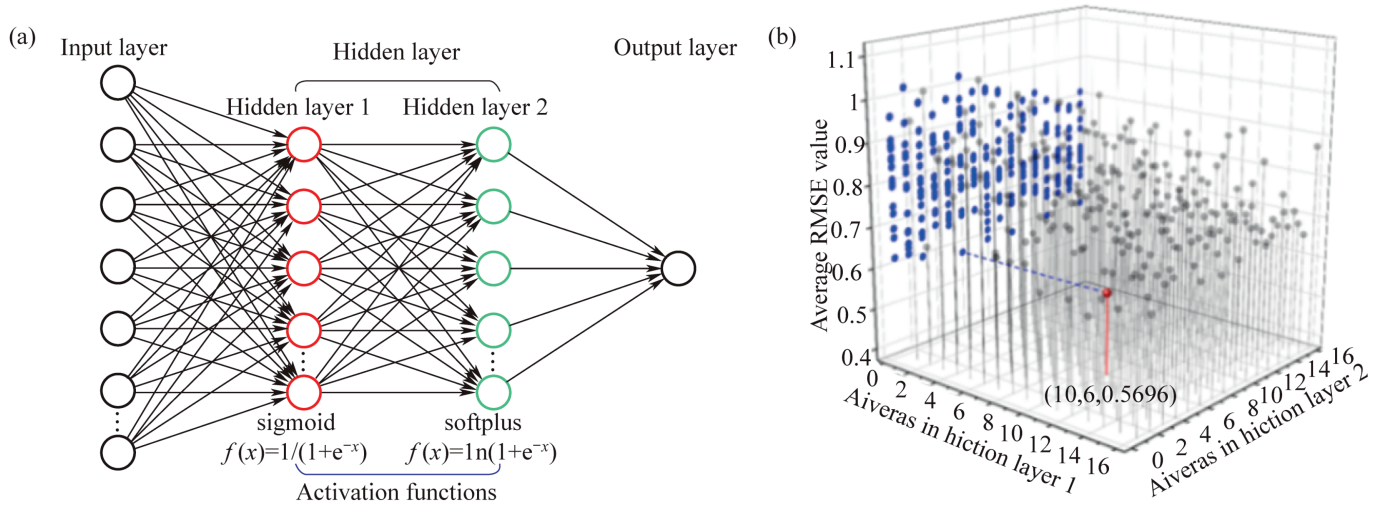

Fig. 3. (a) Configuration of a two-hidden-layer FNN with activation function; (b) average RMSE values from five-fold cross-validation for the FNN model [68], copyright 2021, *Processes*.

influencing toxicity. Simultaneously, 6 styles of interspecies quantitative structure-toxicity-toxicity (i-QSTTR) models were developed to analyze cross-species toxicity responses, providing a theoretical basis for the safe application of ILs [71].

The application of ML in predicting the toxicity of ILs has yielded remarkable results. The constructed models can effectively predict the toxicity of ILs, providing a powerful tool for screening low-toxicity ILs and contributing to the advancement of green chemistry. Future research can further expand the dataset by incorporating more types of ILs and toxicity data under different environmental conditions; delve deeper into the toxicity mechanisms by considering more influencing factors; and continuously optimize model algorithms to enhance prediction accuracy and interpretability. With the continuous advancement of technology and accumulation of data, the application prospects of ML in predicting the toxicity of ILs will become even broader, assisting in selecting safer ILs and assessing potential risks in advance.

3.3. Physicochemical property prediction

ILs have many special physicochemical properties due to their unique structure. Studying the physicochemical properties of ILs is important for acquiring the relationship between their structure and properties, and facilitating the application by unique advantages of ILs. The physicochemical properties of ILs are various, such as viscosity, density, melting point, electrical conductivity, surface tension, and so on, therefore, the relevant research about the properties prediction also accounts for a large proportion. Through the construction of ML models can rapidly and accurately predict their physicochemical properties and conducting in-depth research on these properties helps in designing ILs to meet the requirements of green chemistry and sustainability. Considering the diverse properties of ILs involved, we concluded the details of the research, as well as the numbers of the training and testing data sets, are shown in Table 1 and Table 2.

Table 1
Summary of works using ML methods for prediction of various properties in IL.

Property	IL family	Method	Number of data points or distinct ILs	Training/test set number	Ref.
Melting point	Im, Pip, N, S	DBML, GNN	3080	2464/308	[73]
	Im, N, P, Py	DL, RNN	1253	1002/251	[74]
	Im, Py, Quin, Pyr, Ox, Pip, Mo, Azp, Guan, N, P, S	GNN	/	75%:10%	[75]
Viscosity	Im, Ox, P, Py	LASSO	33	578/72	[76]
	Im, Py, N, P	GP, GMDH	45	2250/563	[77]
	Trz, Pyr, Py, Pip, P, Mo, Im, N, S	KNN, KRR, Lasso regression	/	/	[78]
	Im, N, PIP	ANN, XGBoost, LightGBM	34	1949/414	[79]
	Im, N, Py, Pyr, P, Pip, Mo, S	RF, GB, XGB, GSO	8500	6800/1700	[80]
Electrical conductivity	Im, Trz	FFANN, SVM, SVR, ANN	111	1191/132	[38]
	Im, N, P, S, Pyrr	KNN, SGB, Ada-DT, Ada-SVR	225	2100/525	[81]
	Im, Py, N, P	GNN,RF, DT, GBRT	414	4560/1140	[82]
	Im, Py, N, Pyr	QSPR, RF	577	1951/217	[83]
Surface tension	Trz, Pyr, Py, Pip, P, Mo, Im, N, S	RF, MLP	289	1734/434	[84]
	Im, Py, N, P	ANN, PSO-SVM, LSSVM	62	1136/243	[85]
	Im, Py, N, Pyr, Pip	KNN, GA, PSO, FOA	69	/	[86]
	Im, N, P, Py, Pyr, S	DT, GPR, SVR	69	/	[87]
	Pyr, Py, Pip, P, Mo, Im, N, S	ANN-GC	138	3562/1012	[88]
Density and heat capacity	Im, Py, Pyr, P, N, Pip, Mo, Quin, S	ANN-GC, XGBoost-GC, LightGBM-GC	288 (for density), 31 (for heat capacity)	15248/3191 (for density), 1527/307 (for heat capacity)	[89]
	Quin, Im, Py, N, Pyr, Pip	ANN-GC	17 (for heat capacity), 129 (for density)	1601/353 (for heat capacity), 24282/5335 (for density)	[90]
	Im, Py, N, P	ANN-GC, XGBoost-GC, LightGBM-GC	28 (for density)	7367/1593	[91]

Table 2
Explanation of cations abbreviations presented in Table 1.

Cation names	Cation names
Im: Imidazolium	Py: Pyridinium
Quin: Quinolinium	Pyr: Pyrrolidinium
Pyrr: Pyrroline	S: Sulfonium
Ox: Oxazilidinium	Pip: Piperidinium
P: Phosphonium	Guan: Guanidinium
Mo: Morpholinium	N: Ammonium
Trz: Triazolium	Cs: Cyclic sulfonium

ILs hold immense potential in the realm of energy storage applications and serve as promising candidates for supporting electrolyte materials. The melting point and viscosity of the solvent are pivotal in determining the operational efficiency of the device. However, the practical deployment of numerous ILs remains constrained due to inferior transport properties stemming from their high melting points and viscosity. To efficiently predict the melting point and viscosity of ILs, intelligent prediction methods must be integrated with a thorough investigation of their structural properties [72–74]. Thus, ML models offer a powerful solution. Feng *et al.* [73] proposed descriptor-based machine learning (DBML) and GNN models for IL melting point prediction, with GNN models outperforming DBML ones, and the graph convolutional model showing the best performance, along with an interpretable GNN model revealing atomic contributions. Acar and colleagues [74] used deep learning with recurrent recursive neural networks (RNNs) to predict the melting points of 1253 ILs, selecting key molecular descriptors and achieving high accuracy, while also analyzing descriptor impacts on melting points. Baran *et al.* [75] explored how GNNs process structural information in predicting IL properties like density, viscosity, and surface tension, offering new insights into the relationship between IL structure and melting points. In addition, several researchers have developed predictive models for IL viscosity using different methods and databases. Beckner *et al.* [76] leveraged publicly available data from the IL Thermo database, along with open-source software toolkits such as PyChem, RDKit, and SciKit-Learn, to develop a predictive model for IL viscosity. The model exhibited excellent performance on the validation set, with an mean squared error (MSE) of $4.7\times 10^{-4} \pm 2.4 \times 10^{-5}$ Ps·s and an relative absolute average deviation (RAAD) of 7.1 ± 1.3%. It effectively predicted the viscosity of different types of ILs across a wide range of temperatures, pressures, and viscosities. Kiani and colleagues [77] utilized genetic programming (GP) and group method of data handling (GMDH) models, and evaluated the models using R^2, standard deviation (SD), and AARD. The GMDH model with seven inputs achieved the best performance. Ran *et al.* [78] compared kernel ridge regression (KRR), K-nearest neighbors (KNN), and Lasso regression models, with KNN having the highest test score (0.91628) and lowest root mean square error (RMSE), excelling in predicting IL-water mixtures' viscosity. Hyperparameter tuning *via* Tabu search improved performance. Huwaimel *et al.* [80] compared RF, gradient boosting (GB), and XGBoost models, where the RF model had the highest R^2 (0.9971), low RMSE and mean absolute percentage error (MAPE), and sensitivity and SHAP analyses showed IL concentration as the main predictor of viscosity.

In addition, ML has also been widely used to predict other physical properties of ILs, such as electrical conductivity and surface tension. Several research groups have developed different models to predict the ionic conductivity and surface tension of ILs. Dhakal *et al.* [38] used NIST ILThermo Database to create SVM and ANN models for predicting the ionic conductivity of imidazolium-based ILs. The ANN model outperformed the SVM slightly, with higher R^2 values more than 0.99. Using the ANN, the conductivity of [C_1mim][DCA] was predicted at 3.70 S m^{-1}, 30% higher than the database's highest value. Nakhaei-Kohani *et al.* [81] established KNN, extreme gradient boosting (XGB), adaptive boosting-decision tree (Ada-DT), and adaptive boosting-support vector regression (Ada-SVR) models. The KNN model was best based on chemical structure and temperature, and the XGB model was optimal based on thermodynamic properties and temperature. Meanwhile, sensitivity analysis showed factors of temperature and molecular weight affecting conductivity, and the model reliability was confirmed. Chen *et al.* [83] evaluated COSMO-RS-derived QSPR models for predicting IL conductivity. Here, the COSMO-RS is an effective tool based on quantum chemistry models that can predict the thermodynamic equilibrium and chemical properties of liquids, ILs, or liquid mixtures. It takes molecules as many small fragments surrounded by an ideal shielding conductor, and induces the generation of shielding charges opposite to their charged charges, resulting in a charge density. This method can semi-quantitatively or qualitatively predict the properties of substances through molecular structure without relying on experimental data. With the COSMO-RS-derived descriptors, they improved the ML models performance based on RF and XGB, especially for the XGB-boosting model. Subsequently, a series of studies on the surface tension of materials were conducted using ML models. Benmouloud *et al.* [85] collected data including 1623 binary mixtures with ILs and corresponding temperature, IL molar fraction, and COSMO-RS-based descriptors to predict surface tension with ANN, PSO-SVM, and LSSVM models. The ANN with a "trainbr, logsig" topology performed the best. Abourehab *et al.* [86] using the KNN algorithm combined with three metaheuristic algorithms: genetic algorithm (GA), particle swarm optimization (PSO), and fruit-fly optimization algorithm (FOA) for feature selection to build a model for predicting the surface tension. The results showed that the GENETIC-KNN model performed the best, achieving an R^2 of 0.962 and an MAPE of 1.67×10^{-2}. This model validated an indirect relationship between temperature and surface tension, with surface tension decreasing as temperature increases. Obaid *et al.* [87] used a dataset with 45 input features, AdaBoost was combined with GPR, support vector regression (SVR), and DT to build models. GA) was utilized for feature selection and hyperparameter tuning to predict the surface tension of two novel ILs. The results showed that the boosted GPR model performed the best, achieving an R^2 of 0.981 and an MAPE of 1.73×10^{-2}. This model confirmed that an increase in temperature leads to a decrease in surface tension.

Besides, density is a fundamental thermophysical property of ILs. It holds significant importance in industrial production, influencing factors such as raw material selection, equipment specifications, equilibrium states, and cost considerations. Hence, the construction of an accurate density prediction model is crucial for industrial application. Several research groups have developed models combining the GC method with ML algorithms to predict density as well as other properties. Fu *et al.* [89] used the GC method and ANN, XGBoost, and LightGBM to predict the density and heat capacity of IL-water binary mixtures based on a large number of data points. The ANN-GC model performed the best for density prediction, and SHAP analysis showed that the mole fraction of ILs had the greatest impact on density, along with other factors. Liu *et al.* [90] introduced a combined model for forecasting the density and heat capacity of binary systems comprising ILs and organic solvents. The research determined that the ANN model outperformed others, achieving a mean absolute error (MAE) of 0.0049

and an R^2 of 0.9942 in predicting density within the test set. Furthermore, SHAP analysis revealed that the mole fraction of ILs in the binary system had the greatest influence on the predicted properties. Additionally, factors such as the anion and cation skeleton of the ILs, as well as temperature, also influenced density to varying degrees. Lei *et al.* [91] combined the GC method with ANN, XGBoost, and LightGBM to construct models for predicting the density and viscosity of ternary mixtures of ILs, organic solvents, and water. The ANN-GC model performed the best in density prediction, achieving an ultra-high R^2 value, and SHAP analysis revealed that the cation skeleton of the IL had the greatest positive impact on density, with water mole fraction and anion having different levels of impact.

In summary, the ML method has achieved fruitful results in predicting the physicochemical properties of ILs and provides new avenues for a deeper understanding and application of ILs. In the prediction of key physicochemical properties such as melting point, viscosity, ionic conductivity, surface tension, density, heat capacity, *etc.*, a variety of ML models have been widely used. ML not only improves the accuracy and efficiency of predicting the physicochemical properties but also provides a theoretical basis for the design and optimization of ILs, helping to screen out ILs with specific properties to meet the application needs of multiple fields such as green chemistry, energy storage, catalysis, *etc.* Although significant progress has been made so far, there is still a need to further explore better model architectures, feature engineering methods, and multi-property collaborative prediction strategies to deepen the understanding of ILs and promote their practical applications in wider fields.

3.4. Design and screening

ILs have broad application prospects in the fields such as separation, reaction, and energy storage due to their unique physical and chemical properties, structural tunability, and vast chemical space. However, the traditional trial-and-error method relying on experimental testing with a small number of candidates is inefficient and costly when facing numerous possible structures, making it difficult to fully unleash the potential of ILs. Therefore, the rational design and screening of ILs is a crucial link in their application. Here we conclude the methods and models for various research objects of ILs as shown in Table 3.

The computer-aided IL design (CAILD) method can efficiently screen ILs from a large number of potential structures by establishing structure-property models, as shown in Fig. 4 [92]. This method can be divided into two sub-problems: forward structure-property modeling and reverse molecular design. Models are constructed through different molecular representation methods (such as groups or fragments, descriptors or fingerprints, and learned representations) and modeling algorithms (such as classical linear, non-linear, and deep-learning algorithms). Sui *et al.* [93] proposed a high-throughput computational screening method based on multi-scale computer-aid molecular design (CAMD) and ML. Based on the universal-quasichemical functional-group activity coefficients (UNIFAC) model and the absorption heat transformer (AHT) cycle model, considering IL structure, properties, and process limitations, the best ILs were screened from 26360 candidates. This method was used to design ILs suitable for AHT systems, providing systematic guidance for the molecular design of absorption-cycle working pairs.

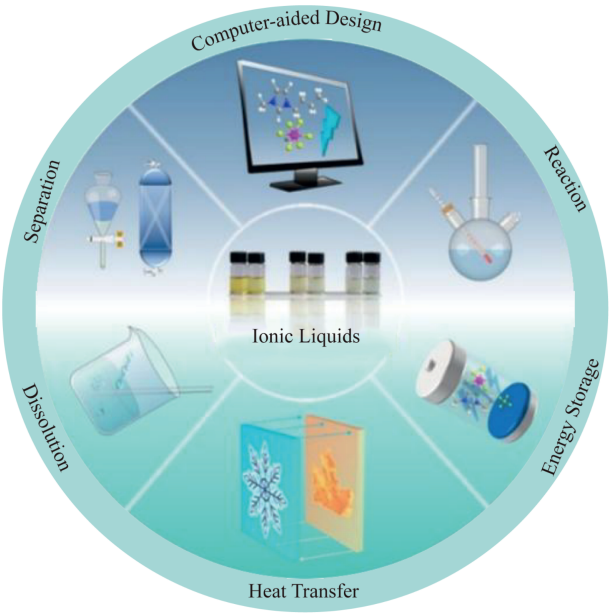

Fig. 4. Representative applications of ILs with CAILD have been reported [92], copyright 2024, *Chemical Reviews*.

In the field of CO_2 capture, ILs are considered as one of the effective substitutes. The design and screening of ILs are the keys to achieving efficient capture. The different methods and models are studied in the recent research. Lemaoui *et al.* [94] proposed a computational method that combines powerful molecular modeling and advanced integrated deep learning to simultaneously predict multiple properties of ILs and achieve eco-efficient inverse solvent design. The COSMO-RS model was used to obtain molecular features, and a DT model was used to evaluate feature importance. The prediction accuracy was improved by adjusting the ANN architecture and introducing a meta-layer. In addition, the syntax-directed variational autoencoder (SDVAE), deep

Table 3
The design and screening of ILs in different research objects.

Research object	Method and model	Ref.
High -profile chemicals	Computer-aided molecular design (CAMD) approach and computer-aided IL design (CAILD)	[92]
Absorption heat transformers (AHTs)	A high-throughput computational screening method, computer-aid molecular design (CAMD) and ML	[93]
Materials science and engineering	The robust molecular modeling and advanced ensemble deep learning method, COSMO-RS model and ANNs	[94]
CO_2 capture systems	SDVAE, DeepFM, and GBPSO models	[95]
CO_2 capture systems	A deep learning-based group contribution framework (DNN-GC and ANN-GC)	[96]
CO_2 separation from flue gas	SVM and GC methods	[97]
Styrene waste gas treatment	Aspen Plus simulation, COSMO-RS model, and transformer-CNN	[98]
Absorption heat pumps (AHPs)	A multi-criteria approach, ML, UNIFAC methods, cycle models, and heat exchanger models	[99]
Electrolytes or solvents	Molecular design model based on variational auto-encoder (VAE), multi-layer perceptron (MLP), and particle swarm optimization (PSO)	[100]
Benzene extraction	QSPR models	[101]
IL-IL binary mixtures	The GC method with three ML algorithms: ANN, XGBoost, and LightGBM	[102]

factorization machine (DeepFM), and gradient-based particle swarm optimization (GBPSO) models form a novel ML method, which were proposed from three key links: molecular generation, property prediction, and optimization, as shown in Fig. 5 [95]. SDVAE converted the molecular structure of ILs into chemical space coordinates and ensured the validity of the generated molecules through syntactic and semantic constraints. The reconstruction accuracies of anions and cations were as high as 99.0% and 98.8% respectively, and the random selection validities could also reach 82.5% and 80.3%, respectively. DeepFM integrated the feature-crossing ability of factorization machine (FM) and the non-linear learning ability of MLP, and accurately predicted the solubility differences of ILs, with an MSE of only 0.00713. GBPSO combined the randomness of particle swarm optimization and gradient correction, effectively avoiding getting trapped in local optimal solutions, and successfully screened out ILs with high CO_2 solubility differences. Mohammed *et al.* [96] constructed a deep learning-based group contribution framework for the targeted design of ILs. This framework could accurately predict the properties of ILs and effectively screen out ILs with high CO_2 absorption capacity, providing a new method for the application of ILs in the field of CO_2 capture. Wang *et al.* [97] established a melting-point prediction model for ILs based on SVM and the GC method, and through this model and other rational design processes, the best IL for separating CO_2 from flue gas was screened out effectively.

In the field of styrene waste gas treatment, ions from COSMO-base2022 were collected to construct a candidate database [98]. The COSMO-RS model was used to calculate the solubility of styrene in ILs, and the absorption and desorption capacities were evaluated. The absorption-desorption process performance of the screened ILs was evaluated using Aspen Plus simulation. The results showed that the ILs obtained through large-scale computational screening outperformed those only considering commercial availability in terms of performance, and this method can be extended to other separation processes.

Faced with absorption heat pumps (AHPs) in renewable and waste heat recovery towards carbon neutrality, Sui *et al.* [99] studied a multi-criteria approach based on ML models, UNIFAC methods, cycle models, and heat exchanger models. The comprehensive evaluation was carried out on 214 new refrigerant/IL working pairs from aspects such as cycle performance, heat transfer performance, hydraulic resistance, and applicable range. In addition, as extractants replacing traditional organic solvents, screening suitable ILs is challenging. Liu *et al.* [100] proposed an IL molecular design model based on variational autoencoders (VAE), MLP, and PSO. This model could achieve multi-objective optimization on a small dataset and effectively solve the problems faced by traditional models in IL design. Amereh *et al.* [101] used the QSPR models to screen ILs for the extraction of benzene from fuels. By collecting 112 liquid-liquid equilibrium (LLE) data of ternary systems containing ILs, benzene, and aliphatic hydrocarbons, the GA was used to select appropriate molecular descriptors, and linear and non-linear QSPR models were constructed. The study showed that considering anion and cation descriptors can significantly improve the model's ability to predict the distribution of benzene between different phases, while aliphatic hydrocarbon descriptors have a relatively small impact. The final linear model could reasonably and accurately estimate the target properties, providing a powerful tool for the screening of ILs.

The design and screening of ILs is a systematic process that needs consideration of the optimal combination of multiple properties simultaneously. The structural and property diversity of ILs makes data acquisition and feature extraction difficult and also puts forward higher requirements for the application of intelligent models. In the future, the combination of various models may be an effective solution.

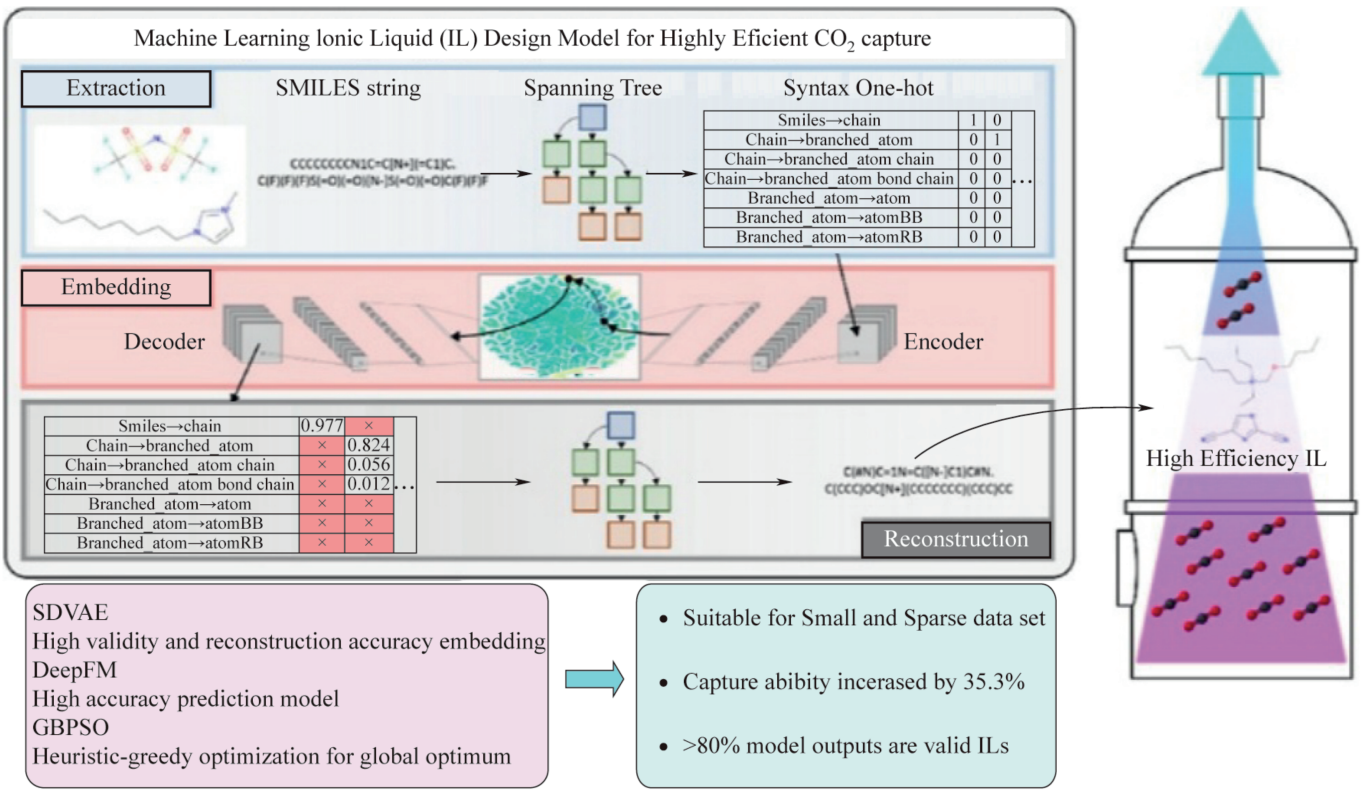

Fig. 5. The application of SDVAE, DeepFM, and GBPSO models in the field of CO_2 capture [95], copyright 2023, *ACS Sustainable Chemistry & Engineering*.

4. Application of Machine Learning on Prediction of Deep Eutectic Solvents

The DESs have many characteristics similar to ILs and have shown broad applications in the fields such as green chemistry, catalytic reactions, material synthesis, and so on. The prediction of properties and intelligent screening of DESs are also important. Nowadays, significant progress has also been made in intelligent prediction according to DESs. In this section, we will mainly summarize and describe the prediction of solubility and physicochemical properties, as well as the design and screening of DESs.

4.1. Solubility prediction

In the fields of chemical engineering, DESs have garnered considerable attention due to their distinctive physicochemical properties. Typically composed of HBDs (*e.g.*, polyols, urea, carboxylic acids) and HBAs (*e.g.*, quaternary ammonium salts such as choline chloride) in binary or ternary systems, DESs exhibit advantageous characteristics including low melting points, cost-effectiveness, and reduced toxicity, *etc*. [14,103]. Recognized as sustainable solvent system [104], these green solvents are demonstrated to be broad applicability in pharmaceutical extraction, gas capture applications, electrolyte, *etc*. Recently, DESs have attracted growing interest in pharmaceutical applications due to their unique solvation properties such as low volatility and tunable chemical microenvironments [105]. However, the vast combinatorial space of DES formulations presents a formidable challenge for the comprehensive screening of optimal solvent systems through conventional experimental approaches. This critical limitation has spurred the development of integrated computational chemistry and ML strategies to accelerate rational solvent design.

In theoretical modeling, researchers have achieved significant advancements by integrating COSMO-RS and quantum chemical calculations with ML algorithms to develop high-efficiency solubility prediction frameworks. Cysewski *et al.* [106] systematically compiled 8014 multi-solvent solubility data points spanning 15 active pharmaceutical ingredients (APIs), innovatively combining COSMO-RS-derived molecular descriptors with ML to optimize 36 regressors (Fig. 6(a)). Their results demonstrated that the nusupport vector regression (nuSVR) model incorporating relative intermolecular interaction parameters and 12-step averaged simplification of σ-potential descriptors achieved optimal performance, representing an improvement in accuracy over conventional approaches. This computational framework constitutes a methodological breakthrough for rational DES solvent design. Further investigations revealed the superior predictive capability of σ-potential-based ML models in specific API systems. Jeliński *et al.* [107] developed predictive models for ferulic acid (FA) solubility in choline chloride/betaine-based DESs, demonstrating that SVR significantly outperformed MLP and standalone COSMO-RS calculations, as shown in Fig. 6(b). This performance advantage stems from SVR's inherent capacity to capture nonlinear relationships in high-dimensional feature spaces. Meanwhile, addressing the solubility-limited efficacy of dapsone (DAP) in therapeutic applications, Jeliński *et al.* [108] employed DESs to enhance its dissolution. Experimental solubility measurements across diverse DESs, combined with COSMOtherm simulations and ML analysis, revealed that DAP self-association constrains solubility, while specific solvent-solute interactions promote dissolution. Through iterative model retraining with expanded datasets, they achieved enhanced predictive accuracy for DAP solubility.

In environmental science and chemical engineering, the efficient capture of industrial exhaust gases and targeted sequestration of hazardous emissions have emerged as critical technological challenges. DESs demonstrate remarkable potential as novel gas absorption media due to their tunable physicochemical properties. Recent studies have systematically investigated DES-based absorption performance prediction mechanisms for industrial gases with both environmental hazards and resource recovery potential, including hydrogen chloride (HCl), nitric oxide (NO), and sulfur dioxide (SO_2), *etc*. through ML modeling approaches. Liao *et al.* [109] established the molar ratio of DES components, hydrogen bond donor/acceptor types, and system temperature as key governing parameters for HCl solubility prediction through dual analytical methods of standardized regression coefficients and Pearson correlation analysis, based on 417 experimental datasets. A systematic comparison of five ML algorithms revealed that a Bayesian-optimized XGBoost model achieved optimal predictive performance, with SHAP value analysis quantitatively elucidating synergistic mechanisms between temperature and acceptor electronegativity on absorption efficiency. Jin *et al.* [110] constructed a multidimensional database containing 292 data points for NO absorption systems, identifying pressure, DES viscosity, and donor hydroxyl group count as core influencing factors through Spearman's rank correlation analysis. The innovative implementation of

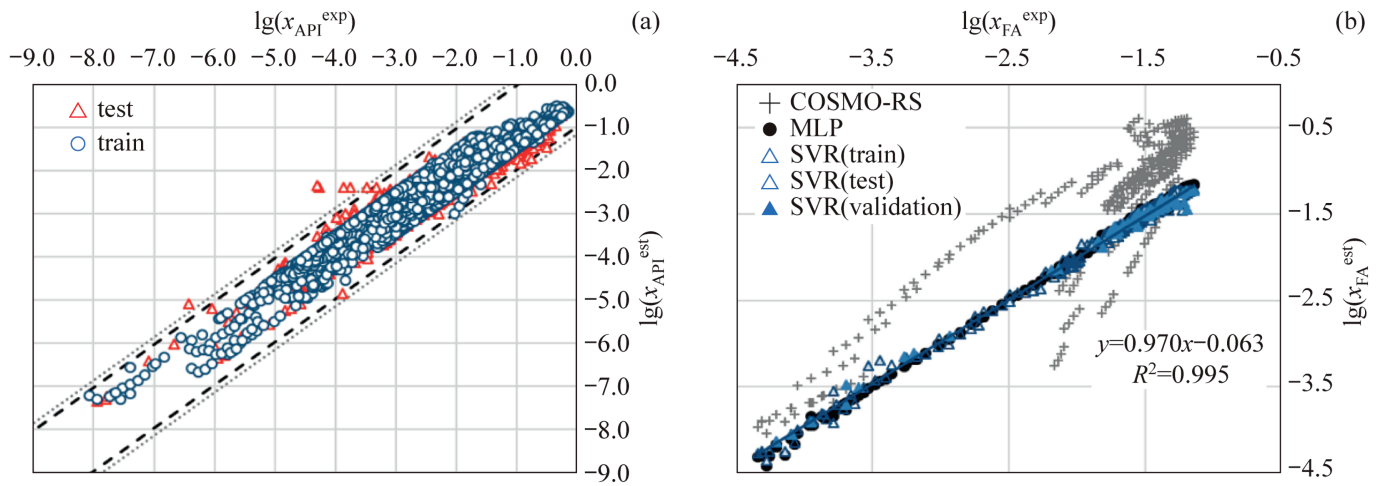

Fig. 6. (a) Error analysis chart of the calculated data by the nuSVR model and the actual solubility of some APIs in DESs [106], copyright 2024, *Molecules*. (b) Correlation between the experimental and calculated solubility of FA in pure, binary, and DESs [107], copyright 2024, *Molecules*.

cascade neural network (CNN) for processing temporal absorption features demonstrated superior accuracy over conventional multilayer perceptron neural network (MLPNN) and recurrent neural network (RNN) architectures. Zhu *et al.* [111] developeda comprehensive gas absorption database by integrating 480 multicomponent DES absorption experiment data. Tri-modal correlation analysis (Pearson/Spearman/Kendall) revealed a strong coupling between DES cavity formation energy and gas polarizability. Comparative evaluation of five architectures identified the Levenberg-Marquardt-optimized MLP model with minimal prediction error, while sensitivity analysis confirmed threshold effects of donor alkyl chain length on SO_2 absorption capacity.

Under the global framework of climate change governance, research on CO_2 capture technologies has emerged as a focal point for both academic and industrial communities. As novel green solvent systems, DESs demonstrate significant advantages in CO_2 capture applications due to their tunable properties and environmental benignity. However, traditional thermodynamic models and COSMO-RS approaches exhibit inherent limitations in predicting the phase behavior of CO_2-DES systems, including restricted prediction accuracy and high parameter sensitivity, which has prompted researchers to explore ML techniques for developing high-precision predictive models [112]. Recent breakthroughs have been achieved in ML applications for solubility prediction in CO_2-DES systems. Mohan *et al.* systematically developed ensemble learning frameworks by ANNs, SVR, RF, and GBT [113,114]. Notably, the ANN-based model demonstrated exceptional predictive performance for 1973 experimental data points covering 132 DESs under varying conditions, while successfully elucidating the impact roles of critical parameters including temperature and hydrogen bond donor-acceptor ratios. Of particular significance, Wang *et al.* [115] innovatively integrated COSMO-RS theoretical descriptors with RF algorithms to establish a QSPR model. This approach achieved superior prediction accuracy across 1011 multidimensional datasets, providing crucial theoretical guidance for DES structural optimization (Fig. 7). In algorithm advancement, Soleimani *et al.* [116] developed a stochastic gradient boosting (SGB) model that reduced the AARD to 0.85%, representing an improvement compared to conventional EoS methods and baseline ML models. Meanwhile, Morales's group [117] made substantial progress through GNN-MG employing molecular graph feature extraction. This architecture demonstrated enhanced generalization capabilities in complex multi-component DES systems, reducing prediction errors compared to conventional ANN and RF models, marking a critical breakthrough in deep learning applications for molecular solvent design.

ML has significantly enhanced the prediction accuracy of solubility for various substances (*e.g.*, APIs, CO_2, and other gases) in DESs by integrating algorithms such as ANN, RF, and GNN with COSMO-RS descriptors and large-scale experimental datasets. This approach effectively deciphers the nonlinear effects of critical variables, including temperature, pressure, and component structural configurations, and helps to deepen the understanding of the interaction mechanism between solutes and DESs, thereby providing an intelligent solution for the high-throughput screening and customized design of DES solvents.

4.2. Physicochemical property prediction

DESs possess attractive physicochemical properties and broad application potential across diverse fields. Despite the remarkable progress in DES research over recent years, their widespread application has been hindered by the limited availability of the amount of data regarding their physicochemical properties. The melting point, density, viscosity, heat capacity, *etc.*, are critical parameters for DESs that significantly influence the suitability for various industrial and scientific applications. Recent advances have indicated the effectiveness of ML approaches in predicting the physicochemical properties of DESs. Hou *et al.* [118] employed the GC method based on a dataset of melting temperatures, which included 1528 DESs and 1541 data points. This method was used to estimate the melting temperatures of binary DESs and ternary DESs with excellent prediction results. Lavrinenko *et al.* [119] pioneered an ML framework for predicting melting points and solid-liquid equilibrium phase diagrams of both DESs and ILs. Their predictive model origin of 1648 melting point measurements across 237 experimentally characterized mixtures, achieved remarkable predictive accuracy compared to previous research. Despite their successful parameterization for aqueous solutions with a focused range of ionic species, COSMO-based models demonstrate significant limitations in their application to more complex systems, particularly DESs or molten salts [120]. The application of these models presents significant challenges in handling the chemical diversity of DES mixtures, especially when dealing with complex systems containing metal-based salts. Ayres *et al.* [121] developed an advanced extreme gradient enhancement model utilizing the XGBoost algorithm, which uses molecular fingerprints, molar ratios, and optimized chemical descriptors as input features for melting point prediction. This comprehensive

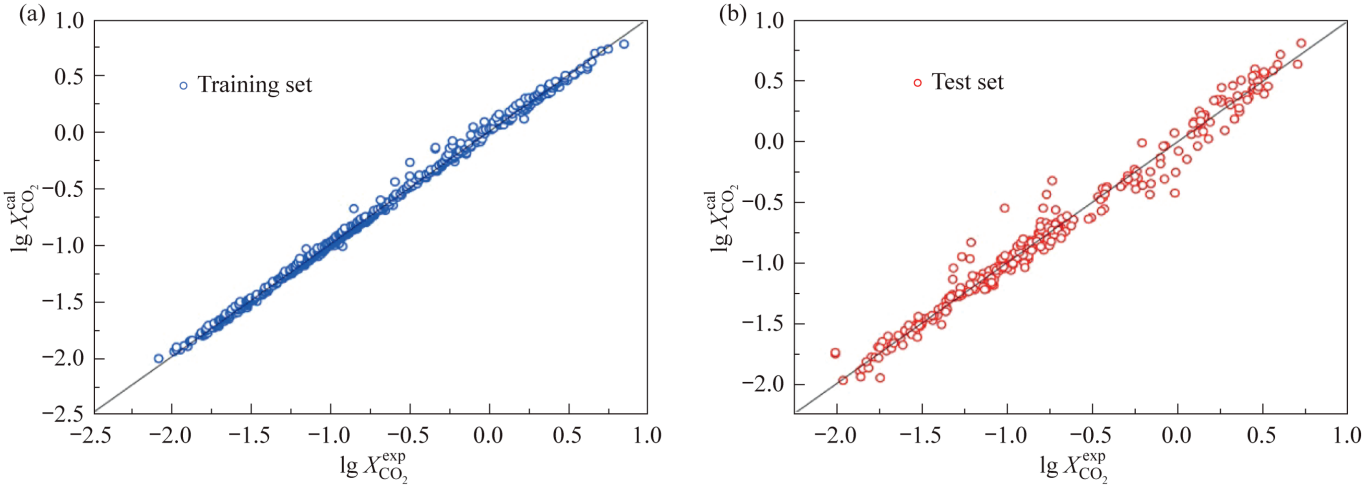

Fig. 7. Experimental and predicted solubility of CO_2 in chemically reactive DES using RF model on training and test sets [115], copyright 2021, *Green Chemical Engineering.*

modeling framework achieved exceptional predictive performance, demonstrating an average accuracy of 97.6% in determining the melting points of DESs (Fig. 8).

The precise determination of volumetric properties in DESs represents a fundamental requirement for the effective design, simulation, and optimization of industrial processes utilizing these solvents. Researchers have developed various predictive models to estimate both the density and viscosity properties of DES systems. Abdollahzadeh *et al.* [122] employed seven ML techniques to estimate the density based on temperature and the inherent properties of DESs, including the acentric factor, critical pressure, and critical temperature. Comparative analysis of 1530 ML estimators revealed that the least-squares support vector regression (LSSVR) model could obtain superior predictive capability, achieving a MAPE of 0.26%. This represented a 74.5% improvement in accuracy compared to state-of-the-art empirical correlations. Roosta *et al.* [123] developed multilayer perceptron artificial neural networks (MLPANN) and LSSVM, which significantly enhanced the density prediction accuracy of DESs through integration with the GC method. Additionally, the predictive ability of the LSSVM-GC model was slightly superior to that of the MLPANN-GC model. Wang *et al.* [124] developed RF models to predict the densities of DESs, using structural information and calculated critical properties as two separate types of features. The findings indicated that the RF models achieve highly accurate predictions for the densities and surface tensions of DESs, with an AARD that was negligible.

Besides, the viscosity of DESs is a key factor because excessive viscosity can impede the rate of heat and mass transfer, ultimately resulting in inhomogeneous heat distribution. However, the measurement of viscosity is time-consuming and laborious, particularly for DESs due to the vast number of possible combinations of HBAs and HBDs. Additionally, the viscosity of DESs is influenced by numerous factors, including temperature, pressure, shear rate, fluid composition, molecular weight, concentration, surface tension, and the presence of additives, making it challenging to predict and control in industrial applications. Shi *et al.* [125] employed several ML algorithms, including SVR, RF, NN, and XGBoost, to predict the viscosity of DESs. Yu *et al.* [126] introduced a novel viscosity equation that correlates viscosity with molecular weight, derived from transition state theory. The energy and structural parameters in this equation were calculated using three multilayer perceptron. The results demonstrated that the transition state theory-inspired neural network (TSTiNet) model overcomes the common limitation of existing viscosity models, which often perform poorly for high-viscosity predictions. The TSTiNet model significantly improved performance metrics, achieving an R^2 value more than 0.98 and a mean absolute relative deviation (MARD) notably lower than those of previous models. Roosta *et al.* [127] developed a hybrid approach to predict the viscosities of a diverse range of DESs by integrating the GC concept with two ML algorithms: the multilayer perceptron (a widely used feedforward artificial neural network) and the LSSVM. Owing to intricate inter- and intramolecular interactions, the viscosity of DES mixtures can markedly diverge from the anticipated values. Hence, it is imperative to devise effective and precise methodologies for screening and forecasting DESs relying exclusively on the structural data of their components. Liu *et al.* [128] employed four ML models to investigate their performance in predicting the viscosity of DESs using extended-connectivity fingerprints (ECFP) with varying lengths as input describers, and the ensemble approach significantly improved the accuracy compared to the best single model. The stacking method leveraged the strengths of each model, combining their prediction results to achieve a more robust and accurate estimation of viscosity.

By leveraging advances in ML, quantum chemistry, and empirical correlations, thereby reducing reliance on experimental measurements and accelerating the discovery and optimization of new materials for chemical processes. Bagherzadeh *et al.* [129] employed the LSSVR with a Gaussian kernel function (LSSVR-G) to predict 503 experimental data points of molar heat capacity. The findings demonstrated that the LSSVR-G model outperforms the existing empirical correlations reported in the literature in terms of accuracy and predictive performance. Khedri *et al.* [130] integrated the MLPANN with LSSVM-GC and LSSVM-AC (AC refers to atomic contribution) methods to predict the atmospheric pressure heat capacities of DESs across a broad temperature range. The developed models exhibited accurate trends without systematic under- or overestimations. Darwish *et al.* [131] employed ML methods, specifically multiple non-linear regression (MNLR) and ANN, to address the intricate molecular interactions within DES systems. The resulting model demonstrated remarkable accuracy and achieving an R^2 value was better than the existing models.

In addition, ML has also been widely applied to predict other physical properties of materials, such as activity coefficients,

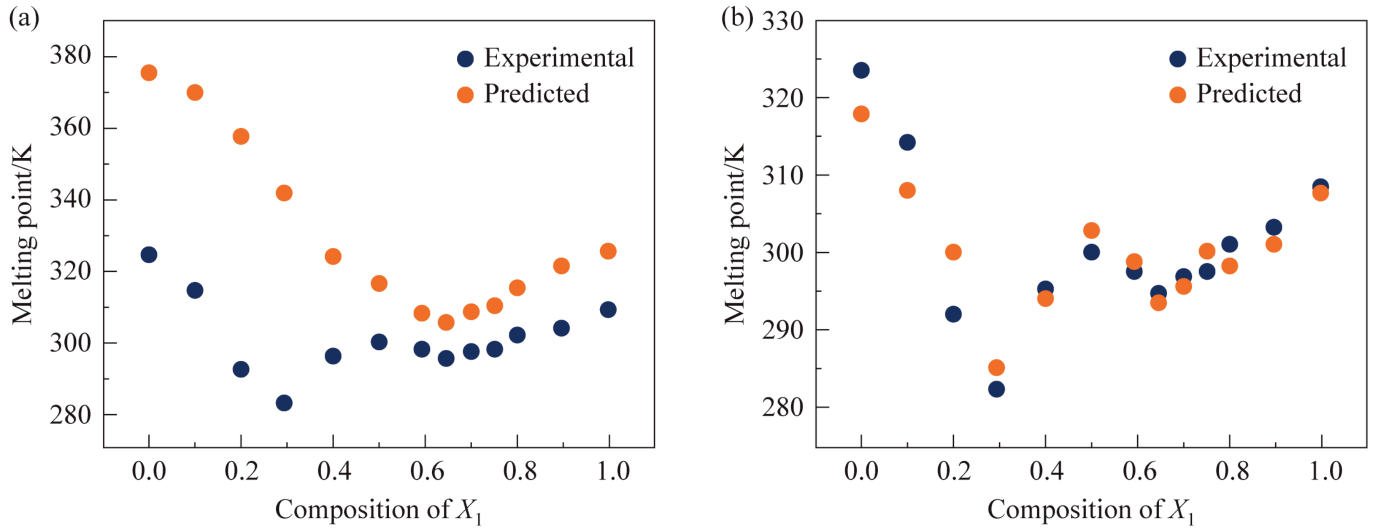

Fig. 8. The experimental and model-predicted phase diagram of $NHex_4I_3/oF_4DIB$ before (a) and after (b) the fine-tuning step [121], copyright 2024, *ACS Sustainable Chemistry & Engineering*.

thermal conductivity, electrical conductivity, *etc*. Abranches *et al.* [132] utilized thermodynamics-informed Gaussian processes (GPs) to precisely model the activity coefficients of various binary mixtures over extensive composition and temperature ranges. Their findings also highlighted numerous adaptable modifications that can be applied to both GP frameworks and active learning (AL) workflows, enabling customization to meet the specific requirements of diverse computational or experimental applications. Li *et al.* [133] developed a predictive model for the infinite dilution activity coefficients (IDACs) of molecular solutes. This model incorporated a comprehensive set of chemical information related to ILs, DESs, and molecular solutes, including chemical functional groups, molecular weights, and Abraham solvation parameters, enabling it to capture both low-order and high-order feature interactions effectively. This approach not only enhanced the accuracy of IDAC predictions but also marked the first time for DESs were included in such predictive models. Additionally, an important DES feature of technology application is its coefficient of thermal conductivity. However, thermal conductivity is not well understood to support reverse design according to technical requirements. Lemaoui *et al.* [134] employed six distinct ML algorithms to predict the thermal conductivities. Among these algorithms, the ANN model, after hyperparameter tuning, delivered the most rapid and accurate prediction results. In addition, solvents were classified to understand the effect of each input on the thermal conductivity of the solvent. The prediction of DESs physicochemical properties using ML methods is summarized in Table 4.

4.3. Design and screening

The intelligent design and screening of DESs are of great significance. Recently, ML models have gained significant traction in the design and screening of DESs. These models leverage large datasets and advanced algorithms to predict the physicochemical properties, stability, and performance of DESs, thereby accelerating the discovery of novel eutectic mixtures with tailored properties for specific applications. Several thermodynamic models have been used in the literature as predictive tools, mainly to identify new eutectic mixtures. These include the UNIFAC, PC-SAFT, and COSMO-SAC methods [135–137]. The COSMO-SAC method, which is based on quantum chemical calculations, has proven to be highly effective in predicting solubility and activity coefficients by accounting for molecular surface charge distributions. By integrating the COSMO-SAC method with ML techniques, a synergistic approach is achieved that efficiently designs suitable DESs. This combination allows for the optimization of DES properties by leveraging the strengths of both quantum chemical insights and data-driven predictive models. Recently, Cysewski *et al.* [138] collected experimental solubility data for a wide range of DES systems. Subsequently, they employed COSMO-RS models to facilitate the rational design and accurate prediction of solubility. This methodology not only streamlined the development of DESs for large-scale applications but also eliminated the need for expensive and time-consuming experimental screening processes. However, the application of the COSMO-RS model has predominantly been limited to predicting solid-liquid equilibria (SLE) of DESs derived from choline chloride, and, its accuracy depends on the specific system, especially the presence of some salts. Ayres *et al.* [139] pioneered the use of transformer models, achieving a satisfactory performance with an F1-score of 0.82. This approach is suitable for predicting a large number of stable eutectic mixtures from a chemical database. Their methodology involved pre-training a transformer model, followed by fine-tuning the final layer of neurons using labeled chemical data specific to natural deep eutectic solvents (NADES) to perform binary classification tasks. This innovative strategy based on the transformer model showed great potential to expand the application of DES

Table 4
Summary of works using ML methods for predicting the physicochemical property of DESs.

Property	Method	Number of data points	Training/test set number	Performance (AARD)	Ref.
Melting point	GGIC (facile group and group-interaction contribution)	1471 (binary DES system)/70 (ternary DES systems)	996/475 (binary DES system)	5.67% (binary DES system)	[118]
	COSMO-RS, SVR	1648	1318/330	/	[119]
	eutXG (extreme gradient boosting)	1648	1240/240	/	[121]
Density	LSSVR, MLP, CFF, GR, RBF, RNN, ANFIS	1239	1053/186	/	[122]
	MLPANN-GC, LSSVM-GC	1410	70%-80% of the data for training set and 20-30% of the data for test set	0.61% for MLPANN-GC and 0.56% for LSSVM-GC	[123]
	RF	3318	2488/830	<1%	[124]
Viscosity	SVR, RF, NN, XGBoost	994	795/199	/	[125]
	TSTiNet, NN	2229	/	6.84% for TSTiNet	[126]
	LSSVM-GC	2533	2026/507	6.88%	[127]
	MLP, RF, GBR, XGB	2217	1477/740	/	[128]
Heat capacity	LSSVR-G	503	428/75	0.27%	[129]
	MLPANN-GC, LSSVM-GC	640	507/133	1.74% for MLPANN-GC and 1.73% for LSSVM-GC	[130]
	ANN	2696	80%-85% of the data for training set and 15-20% of the data for test set	/	[131]
Infinite dilution activity coefficient	DeepFM	52372	/	7.22%	[133]
Thermal conductivity	ANN, DT, GBM, RF, k-NN, MLR	563	461/102	2.17% (ANN), 5.16% (DT), 3.92% (GBM), 4.06% (RF), 3.33% (k-NN), 24.7% (MLR)	[134]

characteristics in different fields. Luu *et al.* [140] extended the model on the Quantum Machines 9 (QM9) dataset to investigate and design key properties of DESs. In addition, they employed an integrated and fully prompt-based multitask generative pre-trained transformer model. This model is capable of solving multiple tasks, including forward prediction, inverse design, and property prediction, and it demonstrated the best overall performance among the approaches tested. GPs are highly versatile and nonparametric models that provide distinct advantages in terms of operation and implementation. Unlike many traditional modeling approaches, this flexibility of GPs allows them to capture complex relationships in data without relying on predefined equations or assumptions about the nature of the interactions. Abranches *et al.* [141] introduced AL methodologies utilizing GPs to efficiently screen nine distinct ternary DESs. By leveraging the inherent ability of GPs to estimate their own uncertainty, the AL framework was employed to decrease the number of data points required for constructing accurate viscosity models, thereby enhancing computational efficiency and reducing experimental effort. As a result, GPs are particularly well-suited for applications where the relationship between variables is unknown or highly nonlinear, making them a powerful tool for predictive modeling and uncertainty quantification in various fields, including ML, engineering, and the physical sciences.

Intelligent prediction and screening have milestone significance for the application of DES and IL, which can effectively reduce experimental workload and accelerate the research and development process. However, intelligent prediction and screening are still in the theoretical research stage, and there is still a certain gap in practical industrial applications. In the future, further exploration of database collection and algorithm improvement is needed to achieve effective and genuine applications in the industry.

5. Conclusion and Perspective

With the rapid development of modern computer technology, intelligent screening and prediction of ILs or DESs through ML has become possible. In this paper, the commonly used ML methods are introduced firstly. Then, the application of the ML models corresponding ILs and DESs is summarized, including the solubility prediction, toxicity prediction, physicochemical property prediction, and the design and screening of ILs and DESs, respectively. Although the research about forecast methods and models for ILs or DESs has been developing for many years, especially in recent years, the application of ML methods is in full swing. However, the research on the application of ML in the fields of the chemical industry is still in the early stages, and there are still many difficulties and problems that need to be explored.

First of all, most of the current ML models applied in chemical engineering are existing and ready-constructed models. The research concerning ML models still stays in the tool stage, and there is no more focus on the algorithm iteration. In the future, the studies should further combine chemical engineering and computer technology in-depth, and more deeply explore the upgrade of the models, even develop new models, making the predicted results more efficient and reliable.

Second, for both prediction and screening tasks, the data determines the upper limit of ML methods. The sufficient quantity and accuracy of the input data is a necessary prerequisite for the effectiveness and feasibility of the constructed ML models. Therefore, the development of high-quality data search and collection technology will be one of the important directions to pay attention to in the future.

Finally, we should take the intelligent forecast method as a medium and further combine it with the theory, simulation, experiment, and advanced equipment effectively, and achieve the really closed-loop research paradigm from the target, to prediction, to screening, to design, and finally to application.

CRediT Authorship Contribution Statement

Yuan Tian: Writing – original draft. Honghua Zhang: Writing – original draft, Investigation. Yueyang Qiao: Writing – review & editing, Writing – original draft. Han Yang: Writing – original draft. Yanrong Liu: Writing – review & editing. Xiaoyan Ji: Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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