Review | Received 10 September 2025; Revised 13 April 2026; Accepted 15 April 2026; Published 6 May 2026
https://doi.org/10.55092/aimat20260004

Advances in adsorption processes driven by machine learning

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Highlights:

- Various algorithms applied to adsorption processes are summarized in detail.
- Different machine learning strategies are analyzed for different adsorption application scenarios.
- The outlook on machine learning in adsorption process applications and challenges is provided.

Abstract: Machine learning, as an advanced data processing method, has become one of the key technologies in the research of adsorption processes due to its outstanding nonlinear modeling capabilities. Its significance lies in that machine learning not only can accurately predict the adsorption process but also plays an important role in the selection and optimization of material synthesis pathways. Currently, research in the field of adsorption mainly focuses on the design of adsorbents, the optimization of adsorption processes, and the development of reactors. This paper systematically classifies the role of artificial intelligence algorithms in adsorption research and reviews the specific applications of these algorithms in the adsorption process, including the screening and design of adsorbents, the prediction and modeling of adsorption parameters, and the design and manufacture of reactors. Machine learning models are classified according to different application scenarios, covering various algorithms such as data modeling, image processing, and sequence analysis. At the same time, this paper also emphasizes the progress made in developing interpretable models for adsorption processes. Finally, the paper discusses the future potential and challenges of artificial intelligence in the field of adsorption.

Keywords: machine learning; process prediction; nonlinear modeling; adsorptive material; adsorption application

1. Introduction

The process of adsorption has long been recognized as a cornerstone and driving force within the chemical industry, with energy consumption for separation and purification accounting for an estimated 45% to 60% of the sector's total energy expenditure [1–3]. As a highly effective separation method based on physical or chemical adsorption, the adsorption process has found widespread applications in

various fields, including chemical engineering, pharmaceuticals, and environmental engineering. biological engineering. Amidst the growing industrial demands and the global surge in commitment to environmental sustainability, as evidenced by the United Nations' reports on the progress of sustainable development goals, the exploration of adsorption separation technologies is poised to seize unprecedented opportunities while navigating significant challenges. Within this evolving context, the imperative to enhance the efficiency and precision of adsorption processes through innovative technological breakthroughs has emerged as a central concern for the chemical industry [4,5].

In the domain of adsorption separation, the development and optimization of adsorption models represent a crucial focus of contemporary research [6,7]. Historically, research in this area has primarily depended on the gathering of empirical data and the construction of classical theoretical frameworks. These methodologies have been instrumental in enhancing researchers' comprehension of the fundamental principles underlying adsorption processes and clarifying the interactions betwbetween adsorbents and adsorbates, thereby facilitating the preliminary optimization of adsorption systems. For instance, classical models such as the Langmuir and Freundlich isotherms, grounded in physicochemical assumptions regarding adsorption phenomena, have provided a solid theoretical foundation for characterizing the adsorption behavior of adsorbent surfaces toward target substances [8,9]. Simultaneously, advancements in theoretical approaches, including molecular dynamics simulations, have yielded critical insights into the intricate microscopic mechanisms that govern adsorption processes [10].

In practical applications, adsorption separation systems frequently exhibit non-linear characteristics, as evidenced by the non-linear adsorption isotherms and the impact of non-linear adsorption on ion exchange processes. For example, in multicomponent systems, competitive interactions among components can significantly alter adsorption behavior, as evidenced by studies on solute-surface interactions, competitive adsorption in rare earth ores, and the adsorption kinetics of VOCs on resins. In dynamic adsorption processes, factors such as variations in mass transfer resistance, pore structure, and operational conditions frequently interact in a highly coupled and intricate manner, further complicating system performance [11,12]. These multifaceted challenges highlight the limitations inherent in traditional experimental and theoretical methodologies. Experimental approaches frequently require significant investments of time and resources, whereas classical theoretical models often face challenges in balancing precision with broad applicability in complex systems.. This limitation is particularly pronounced in large-scale industrial applications, where traditional modeling techniques frequently fail to deliver rapid and optimization strategies [13]. As a result, these constraints have, to a certain extent, hindered the further advancement and widespread adoption of adsorption separation technologies [14].

With the rapid development of AI (artificial intelligence) technology, especially the rise of data-driven methods such as machine learning and deep learning, the research of adsorption separation technology has brought revolutionary changes [15,16]. By learning and analyzing large amounts of data, artificial intelligence can easily handle complex nonlinear problems that are difficult to solve using traditional methods, and demonstrates strong capabilities in modeling, optimization, and the application of adsorption separation. In particular, the machine learning algorithm can identify underlying principles and significant factors influencing adsorption by leveraging experimental and simulated data, offering a dependable approach for forecasting adsorption efficiency and refining process methodologies.

Simultaneously, AI offers the potential to substantially improve both the efficiency and precision of adsorption process research. Traditional experimental investigations often necessitate meticulous

adjustments across a multitude of interdependent variables, including the specific surface area of the adsorbent, pore size distribution, molecular properties of the adsorbate, and operational conditions such as temperature and pressure. For instance, nanoscale structures, with their unique physical and chemical properties, can significantly influence adsorption efficiency. The surface area and pore size distribution of the adsorbent are critical factors, as they determine the number of available adsorption sites and the accessibility of the adsorbate molecules. Additionally, the molecular properties of the adsorbate, such as size, polarity, and chemical structure, play a pivotal role in the adsorption process. Operational conditions, including temperature and pressure, also have a profound impact on adsorption efficiency, as they can affect the kinetic and thermodynamic aspects of the adsorption process. In stark contrast, AI models, powered by advanced algorithms and substantial computational capabilities, can swiftly execute global searches and optimize parameters, markedly reducing the time and effort involved in these investigations. For instance, when hyperparameter optimization techniques are integrated with machine learning algorithms, they can rapidly determine the optimal operating conditions for adsorption processes, thereby significantly improving separation efficiency. Furthermore, AI-driven methods for modeling complex systems adeptly integrate experimental data with theoretical frameworks, enabling researchers to overcome the inherent constraints of traditional methodologies and explore new realms of understanding. Notably, the integration of artificial intelligence in adsorption separation not only enhances operational efficiency but also drives the technology towards higher sophistication and precision. From an intelligence perspective, real-time monitoring and adaptive regulation of adsorption processes can be realized through the deployment of online sensors that capture critical parameters—such as temperature, pressure, and flow rate within adsorption towers. These data are dynamically analyzed and predicted by AI models, establishing a foundation for autonomous and optimized system control.

While AI has brought numerous benefits to adsorption separation research, it still encounters certain challenges in practical applications. A major obstacle arises from the intrinsic characteristics of many AI algorithms, especially complex models like deep learning, which are frequently labeled as “black box” systems. This description stems from the challenge of interpreting or intuitively grasping the internal mechanisms and decision-making processes of these models. Consequently, their effectiveness in specific tasks primarily depends on the correlations between inputs and outputs, rather than a deep understanding of the underlying physicochemical mechanisms.

To tackle these challenges, integrating AI algorithms with the empirical knowledge inherent in traditional adsorption disciplines has become a key strategy for improving both the efficiency and accuracy of adsorption separation processes. This approach serves as a crucial pathway for advancing the field into an era of enhanced intelligence and precision. By combining the strengths of both methodologies, this synergy not only enhances the interpretability of AI models but also facilitates a deeper integration of theoretical principles with data-driven approaches, thereby charting new directions for adsorption separation research [17,18].

This work underscores the significance of integrating domain knowledge from adsorption science into machine learning models, ensuring compliance with physical constraints and theoretical relevance while harnessing the advantages of data-driven approaches. This synergy empowers researchers to discover new insights and overcome traditional constraints, thus promoting innovation. Current research in adsorption focuses on three key areas: adsorbent design, adsorption process optimization, and reactor development. The paper systematically categorizes AI algorithms based on their roles and reviews their

applications throughout the adsorption process, including adsorbent screening and design, prediction and modeling of adsorption parameters, and reactor design and fabrication. Machine learning models are classified by application scenarios, such as data modeling, image processing, and sequence analysis. Progress in developing interpretable models specifically tailored to adsorption is also highlighted. Finally, the paper explores the future potential and challenges of AI within the field of adsorption, proposing innovative ideas—such as the integration of adsorption processes with 3D printing technology—to inspire further advancements in this domain.

2. Data collection and resources for adsorption-ML research

The utilization of AI and technology in the investigation of adsorption mechanisms presents distinct advantages. AI has the capability to automatically optimize the cross-scale parameter design of adsorption materials based on experimental data and generate a structural model with optimal adsorption performance. It can rapidly materialize the design scheme optimized by AI, fabricate a cross-scale adsorption structure, and validate the accuracy and practicality of the AI model through experiments. Leveraging AI's proficiency in modeling complex problems, the internal relationships between micro and macro scales can be explored. This serves to guide researchers in establishing novel mechanisms for mass and heat transfer processes at different scales.

In recent years, many papers on AI + adsorption have been published. It is impossible to select them all here. By searching for articles in Web of Science using the keywords "adsorption" and "machine learning" with a time limit of the past five years, approximately 2300 non-review articles were found. Then, further searching was conducted using the keyword "MOF synthesis", and 22 papers were obtained. Among them, 5–6 representative papers were selected. Additionally, based on the keywords "adsorption" and "machine learning", searching with the keyword "high-throughput screening" yielded around 180 papers. Then, 5–6 papers with higher impact factors were selected. Similarly, the keywords "reactor design", "Reactor simulation", "adsorption energy model", *etc.* were used for keyword search. Due to the similar content reporting processes of many literature, the journals with higher impact factors were selected for description.

As shown in Table 1, a systematic review of research on the application of machine learning (ML) in fields such as material design, adsorption performance prediction, reaction optimization, and process monitoring reveals that ML technology exhibits significant application potential in improving R&D efficiency, optimizing system performance, and enhancing model interpretability. Analysis indicates that there are substantial differences in the training sample sizes among different models, with the sample scale ranging from approximately 100 to 600,000. This variation is primarily determined by the difficulty of data acquisition: tasks related to material screening and performance prediction typically rely on larger sample sizes (e.g., tens of thousands to hundreds of thousands of samples), and the core reason lies in the fact that an adequate sample size is a prerequisite for accurately capturing the intrinsic properties of materials. Although deep learning models can achieve high-precision predictions, they have higher demands on data scale, which is closely associated with the mechanism of such models extracting complex features through multi-layer nonlinear transformation. Further observation shows that the application proportion of graph neural networks (GNNs) and interpretable AI models has increased significantly. This is attributed to the fact that while maintaining prediction accuracy, these models can reveal key factors affecting adsorption performance (e.g., material topological structure, surface chemical properties, *etc.*), providing interpretable quantitative basis for mechanism analysis and performance optimization.

Table 1. Summary of the AI + adsorption process.

No.	Task	Type of data	Input features	Dataset Size	ML Algorithm	CV Strategy	Best Performance Metric	Improvement *vs.* Baseline	Reference
1	Predict selectivity for high-purity C_3H_6	Adsorption-related data of MOF for C_3H_8/C_3H_6	Energy descriptors: (ΔQ_{st}, S °); Structuraldescriptors: (PLD, LCD, GCD, ASA)	Not mentioned	DT, RF, XGBoost, CatBoost (RF best)	Not mentioned	RF's R^2 = 0.83; IAST = 2.7	3-order faster; JNU-90 superior	[19]
2	Enhance MB adsorption & optimization	Adsorption-related data of SAH for pollutant: Eads; q_e; RR_{MB}, structural characterization data, operational parameter data	Quantum chemical: descriptors: (E_{ads}, E_{HOMO}, $E_{LUMO,}$ E_g,χ) Operational parameters: (adsorbent dose, initial MB concentration, solution pH, contact time) structural parameters: (monomer combination, crosslinker concentration, initiator concentration, reaction temperature, stirring rate)	1000+ topologies	Single-hidden-layer ANN (4-14-2)	Not mentioned	Average R^2 = 0.9998	Not mentioned	[20]
3	Predict adsorption, screen optimal materials	Adsorption-related data for gas separation: equilibrium adsorption isotherms, breakthrough curves, τ_b, dynamic loading capacity, selectivity, and adsorbent property data	Bed design parameters: (bed length, void fraction), operating conditions: (feed pressure, feed velocity, feed composition), isotherm parameters: ($b_{i,s}$, $m_{i,s}$, $\Delta U_{i,s,}$ ΔH_i, adsorbent particle density)	10k training, 5k validation, 196 zeolites	Feedforward ANN (35-35-35)	Independent set, select high R^2 model	R^2 = 0.9957 (carbon capture)	33,333 × faster, high-throughput screening	[21]
4	Predict target crystal formation	Hydrothermal reaction data for templated vanadium selenite, including successful and failed reaction records with compositional information, reaction conditions, and reaction outcomes	Organic/oxalate-like reactant properties: (molecular weight, hydrogen-bond donors/acceptors, polar surface area) Inorganic reactant properties: (atomic properties) Experimental conditions: (temperature, reaction duration, pH,) Permutation-invariant descriptors: (max, min, arithmetic/geometric means for each reactant type)	3955 reactions	SVM (main), C4.5 (auxiliary)	2:1 split, 15-time avg validation	SVM 79% accuracy, 89% experimental success	11% higher than human intuition ($P < 0.05$)	[22]
5	Predict phenol adsorption capacity in RP	Phenol adsorption-related data in RPB including input operational parameters and corresponding phenol adsorption capacity	Liquid spray density, initial phenol concentration, gravity factor, contact time.	180 samples (80% train, 20% test)	MR, ANN, SVR (ANN best)	10-fold CV, leave-one-out	ANN: R^2 = 0.9986, RMSE = 0.0273	ANN better than MR, RMSE ↓81.7%	[23]
6	Predict TC/SMX Q on CBMs	Adsorption data of tetracycline and sulfamethoxazole on carbon-based materials, including CBMs properties, adsorption conditions, and corresponding adsorption capacity	CBMs properties: (Total carbon content, H/C, (O+N)/C, ash content, BET surface area, point of zero charge) Adsorption conditions: (Temperature, solution pH; Initial concentration ratio: initial TC/SMX concentration *vs.* CBMs dosage)	111 CBMs, literature data	RF, GBT, ANN (RF best)	8:2 split, 5-fold CV	RF: $R^2 \approx 0.90$	Better generalization than traditional models	[24]

Table 1. *Cont.*

No.	Task	Type of data	Input features	Dataset Size	ML Algorithm	CV Strategy	Best Performance Metric	Improvement *vs.* Baseline	Reference
7	Predict biochar's ECs adsorption capacity	Adsorption capacity data of biochar materials for emerging contaminants in aqueous solutions, including biochar synthesis conditions, characteristics, compositions, and adsorption experimental conditions	Biochar synthesis conditions: (Pyrolysis temperature, pyrolysis time, biochar type;) Biochar characteristics: (BET surface area, pore volume, average pore size) Biochar compositions: (C (%), Ash (%), N/C, H/C, O/C, (O+N)/C) Experimental conditions: (time, temperature, initial concentration, adsorbent dosage, solution pH/volume, pollutant type, rpm, wastewater type, ion concentration, adsorption type)	3757 data points, 24 variables	10 tree-based models (CatBoost best)	7:3 split, 1000-time validation	CatBoost: R^2 = 0.9433, MAE = 4.95	Better than traditional models in data/ performance	[25]
8	Predict 7 MAM part mechanical properties	Mechanical properties data of MAM parts, including processing parameters, material properties, machine types, post-processing conditions, and corresponding mechanical properties	Processing parameters: (Beam power, layer thickness, scanning speed, beam diameter) Material properties: (Density, melting point, thermal conductivity, specific heat, CTE, chemical composition elemental properties) Categorical features: (Material type, MAM process/sub-process, machine type, post-processing condition, specimen orientation.)	1600 data points, multiple variables	8 models (mostly RF best)	5-fold CV, 1000-time validation	RF: $R^2 \approx 0.95$	Better than traditional methods in generalization	[26]
9	Classify MOF stability	MOF stability data, including solvent removal stability and thermal stability; Curated from experimental literature via NLP	Revised autocorrelations (RACs, graph-based fingerprints derived from MOF CIF and geometric features)	2179 (stability), 3132 (Td)	ANN	3-set split, blind test validation	Accuracy 0.76–0.78	Larger data, better accuracy than traditional	[27]
10	Phase identification, content grading	Synthetic and experimental powder XRD patterns of multiphase inorganic compounds in the Sr-Li-Al-O quaternary compositional pool; Labels include constituent phases and phase fractions	1D XRD pattern data consisting of intensity *vs.* 2θ values; Simulated patterns incorporate adjustable parameters: (peak profile, background, white noise) fixed parameters: (multiplicity, polarization correction)	3 synthetic sets + 100 real patterns	CNN (main), KNN/SVM/RF (comparison)	6:1:1 split, real data validation	Phase accuracy nearly 100%	Faster, more accurate than traditional	[28]
11	Automatic recognition of particle size and morphology	SEM images of nanomaterials; Labels include morphology types and manually measured particle sizes	SEM image pixels (raw image data); Image-derived features: (contrast-enhanced regions, binarized foreground/background)	274 classification + 66 measurement images	Inception-V3 (main), basic CNN (comparison)	7:3 split, manual measurement validation	Classification 87% accuracy, 0.99 correlation	Faster, more accurate than traditional tools	[29]
12	Predict highly accurate molecular infrared spectra via machine learning	AIMD data from DFT calculations: molecular geometries, potential energies, forces, and dipole moments of three systems	ACSFs describing the local chemical environment of each atom (dependent on neighboring atom positions and cutoff radius); Used to train HDNNPs and neural network dipole models	245–718 DFT reference configs	HDNNP + neural dipole model	Adaptive sampling, no K-fold CV	Energy MAE 0.048 kcal/mol	3–6 orders faster, high accuracy	[30]

Table 1. *Cont.*

No.	Task	Type of data	Input features	Dataset Size	ML Algorithm	CV Strategy	Best Performance Metric	Improvement *vs.* Baseline	Reference
13	Accelerate adsorption energy calculation for adsorbate-surface systems via machine learning	Adsorbate-surface configuration data from DFT calculations: Initial configuration, relaxed energies, forces, and adsorption energies	Atomic structure representations (used by graph neural networks) describing adsorbate-surface local environments	OC_20-Dense, ~190k configs	GNN	Not mentioned	Success rate 91.61%,	Accuracy near DFT, 2 orders faster	[31]
14	Real-time, *in-situ* monitoring of organic contaminant adsorption	SIP measurements during breakthrough experiments and adsorption-desorption cycles; Dye concentration data for model calibration/validation; Hydraulic and geometric parameters of AC filters	SIP-derived imaginary conductivity values; Used as a proxy for adsorbed dye concentration in reactive transport modeling	No size, experimental monitoring	reaction-transport model	Not mentioned	$R^2 \approx 0.96$-0.98	Real-time *in-situ*"	[32]
15	A machine learning-based real-time monitoring system for smart connected workers in manufacturing; Functions	Visual data: (Image frames from 3 cameras Digital data: (Smart meter readings of manufacturing devices) Labeled data: (Bounding boxes for object detection, ground truth machine states, text labels, and worker interaction gestures)	Object detection: (Image pixels for 3D printer components) Text/finger recognition: (Image pixels for machine panel texts and worker finger positions) Skeleton detection: (RGB image pixels for worker body joints); Energy disaggregation: (Sequential smart meter data)	Object detection: 4400 labeled images Text/finger recognition: 442 test frames Skeleton detection: 12,120 frames	YOLO, CRAFT, LSTM,	Simple split, no multi-fold CV	State prediction accuracy 100%	Faster, more integrated functions	[33]
16	Develop a generalizable computer vision and machine learning system for real-time monitoring and control of chemical workup processes	Raw image pixels from the webcam; Extracted visual cues include liquid volume, homogeneity, turbidity, presence of solids/residue, and color; Integrated with process variables from iControl software	Visual data: (Image frames from a webcam capturing reactor interiors) Process data: (Reactor temperature, stir rate, dosed solvent volume.) Labeled data: (Manually annotated images for model training, capturing chemical/physical processes in reactors)	Pre-trained on COCO dataset + fine-tuned with manually annotated images of chemical processes	Mask R-CNN (core)	No CV, repeated experiment validation	Accurate volume control, phase recognition	Universal, non-invasive, low-cost	[34]
17	Develop a reduced-order model for nuclear reactor primary circuit to accelerate thermal-hydraulic calculations	FOM data: (Thermal-hydraulic simulation results of AP1000 reactor primary circuit components under different operating conditions); Snapshots: (FOM-derived data of key variables from typical operating states) Design parameters: (Reactor core/steam generator design values for model validation)	Key thermal-hydraulic variables from FOM snapshots, including (mass flow rate, momentum, pressure, dynamic viscosity-related terms, enthalpy, and temperature)	Snapshots: 11 operating conditions covering 70%–100% rated power; Validation data: 2 additional operating conditions not included in snapshots	using POD + LSM	case extension validation	Error 0.223%,	Efficient, accurate *vs.* full-order model	[35]

Table 1. *Cont.*

No.	Task	Type of data	Input features	Dataset Size	ML Algorithm	CV Strategy	Best Performance Metric	Improvement *vs.* Baseline	Reference
18	Develop a machine learning-based approach to optimize single-channel design of molten salt reactors	Training/test data: Neutronic simulation results of MSR single-channel configurations	feature parameters: (Fuel type, salt type, uranium content, channel spacing, moderator/salt volume ratio, average temperature)	285k training, 8k test samples	ET best, including RF, SVM, *etc.*	Test set validation, no multi-fold CV	R^2 = 0.99, error < 5%	Higher efficiency, better accuracy	[36]
19	Develop a CFD based multi objective Bayesian optimization tool for chemical reactor design	CFD simulation data: (Effective gas holdup and power consumption of reactor configurations;) Design parameter data: (Discrete values of 6 reactor design variable)	Six discrete design variables: (Tank aspect ratio, lower impeller clearance ratio, upper impeller clearance ratio, sparger-impeller diameter ratio, impeller-tank diameter ratio, sparger height-lower impeller clearance ratio)	80 valid CFD simulation samples	Multi-objective Bayesian optimization (MBO)	No CV, convergence validation	Power ↓85%, gas holdup ↑95%	Higher efficiency, better performance	[37]
20	Develop a combined CFD, machine learning, and response surface methodology approach to optimize ammonia decomposition in a porous catalytic shell-and-tube reactor	CFD simulation data: (Ammonia conversion, system efficiency, hydrogen mass flow rate, and pressure drop of reactor configurations); Model validation data: (Experimental and numerical ammonia conversion data for CFD model calibration); ML/RSM data: (Input variables and corresponding performance metrics for model training, validation, and optimization)	Eight variables: (Pore diameter, porosity, tube convection heat transfer coefficient, reactor inlet temperature, tube inlet temperature, reactor inlet velocity, tube inlet velocity, and foam thermal conductivity)	287 sets (110CFD+177ANN)	BRNN + RSM (CCD design)	7:1.5:1.5 split, CFD validation	ANN R^2 > 0.99, error < 14.38%	Higher efficiency, H_2 yield × 6.45	[38]
21	Develop a machine learning-aided CFD approach to facilitate design of experiments for CO_2 capture reactor	CFD simulation data Experimental data Model calibration data	Benchmark optimization: (Inlet velocity, bed thickness; Temperature-varying modeling: Adsorption rate coefficient, desorption rate coefficient, time shift)	331 CFD sets, temp-dependent data	Kernel Ridge Regression (KRR), Neural Network (NN)Optimization: Bayesian optimization; Calibration: Bisection method.	Proportional split, physical validation	RMSE = 0.0048	Faster, lower data demand	[39]
22	Develop an uncertainty-aware adaptive DT for pressure swing adsorption PSA systems	Synthetic data Operational data Model calibration data	Eight operational variables: (Feed time, purge time, rinse time, high pressure, low pressure, rinse flow rate, purge flow rate, inlet temperature)	50k LHS samples + degradation data	DNN(NARX)+MCMC+OL	No CV, multi-dimensional validation	Error < 1% at 20% degradation	Adaptive, uncertainty-aware	[40]
23	Develop a software tool concept for rapid and flexible creation of mechanistic DT core models for bioprocesses	Experimental data Simulation data Parameter data	Biokinetic inputs: (Substrate concentration, biomass concentration, enzyme concentration); Physico-chemical inputs: (Temperature, pH, dissolved oxygen, foam level; Reactor inputs: Reactor configuration, flow rates, volume, aeration rate, stirring rate)	16 parameters + 1 validation datasets	No ML, using mechanistic modeling	No CV, experimental validation	Development/ computation time 90%, $R^2 \approx 0.9$	Faster, more flexible	[41]

Table 1. *Cont.*

No.	Task	Type of data	Input features	Dataset Size	ML Algorithm	CV Strategy	Best Performance Metric	Improvement *vs.* Baseline	Reference
24	Develop a physics-based digital twin framework for combustion devices by integrating CRN and sparse sensing	CFD simulation data CRN data Operating condition data	Operating parameters:(Rich zone equivalence ratio, air preheating temperature, fuel hydrogen content, operating pressure)	15 baseline + 7 extended CFD datasets	GPR (comparison), POD auxiliary	No CV, sub-domain validation	Extrapolation NRMSE ≈ 10%, faster than CFD	Better extrapolation, physically consistent	[42]
25	Develop a digital twin platform for a four-bed two-evaporator adsorption chiller system	Experimental data; Simulation data; Case study data	Fourteen operating parameters: (Hot water inlet temperature, cooling water inlet temperature, low/high-pressure evaporator chilled water inlet temperatures, mass flow rates of hot/cooling/chilled water, operating times)	≥ 20 experiments + 50k optimization data	No ML, using ASO optimization	No CV, experimental validation	COPth 9.6%, power 10.3%	Better performance, lower energy	[43]
26	Develop an interpretable machine learning-guided strategy to break adsorption-energy scaling limitations for electrocatalytic nitrate reduction reaction to ammonia	DFT calculation data Experimental data Isotope labeling dat	Catalyst-related features: (Surface face, metal composition, electronic structure, interlayer spacing;) Reaction-related features: (Adsorption energies of $*NO_3$(bridge-bidentate) and *N(hollow), applied potential)	≥ 50 ML + multiple DFT/experiments sets	Bayesian chemisorption theory	No CV, DFT/experimental validation	FE 92.5%, yield 6.25 mol/(hg)	reaks scaling, 2 ×better performance	[44]
27	Develop a Transformer-based Uni-MOF for high-accuracy gas adsorption prediction in MOFs and COFs	Structural data Adsorption data Experimental data: Structural feature data	Material features:(3D atomic coordinates, lattice matrix, atom types from CIF files;) Gas features:(Gas ID, intrinsic descriptors); Operating condition features: (Temperature, pressure)	631k structures + 3M adsorption points	Improved Transformer (self-supervised pre-train)	8:1:1 split, cross-system validation	R^2 = 0.98,	10^4 × faster, better generalization	[45]
28	Predict CO_2 uptake in biomass-waste derived porous carbons (BWDPCs) using ML models	Scientometric data Experimental/literature data Target variable	Material properties:(SA, TPV, MPV, elemental contents; Operating conditions: (Temperature, pressure)	439 sets (351 train + 88 test)	XGBoost best, ANN/DT/RF comparison	8:2 split, visualization validation	XGBoost test set R^2 = 0.86	Higher accuracy, strong interpretability	[46]
29	Identify key physical quantities determining chemisorption energy on binary alloy surfaces using AutoML-based feature deletion experiments	DFT data: Feature data Test data.	Physical feature (polarizability) Molecular descriptors (geometric characteristics + Physical and chemical characteristics)	439 sets (351 train + 88 test)	GPR best, MLP/RF/ERNN comparison	multi-metric validation	Test set R^2 = 0.98, RMSE = 0.14	Higher accuracy, strong interpretability	[47]
30	Predict excess hydrogen uptake of porous carbon materials using machine learning		Textural features: (BET, total pore volum, micropore volum, ultramicropore volume); Chemical features: (C, hydrogen H, O, N content); Operating feature: (Pressure)	1745 data points (68 materials)	RF best, LR/SVR/XGBT comparison	Group 5-fold nested CV, Bootstrap validation	RF's R^2 = 0.91, MAE = 0.414	Accurate quantification, resolve literature conflicts	[48]
31	Predict the static water contact angle (CA) of polymer brush surfaces as an indicator of hydrophilicity/hydrophobicity using machine learning	Experimental/ literature data Material property data Operating condition data	physical feature: (Polymer thickness) molecular descriptors: (MaxPartialCharge, MinPartialCharge, Hydrogen bond acceptor, hydrogen bond donor, number of heteroatoms)	100 data points (38 materials)	SVR best, 8 models compared	Nested 5-fold CV, external validation	External validation CA error < 3 °	Quantitative prediction, explains mechanism	[49]

In general, the application of ML in the fields of materials and chemical engineering has gradually advanced from the stage of qualitative description to that of quantitative verification. However, existing studies still have common issues: the cross-validation strategies in some works lack standardization (e.g., failure to clearly specify the validation method or number of repetitions), and the comparative experiments with baseline models are insufficient, which limits the comparability and reliability of the results. Future research should focus on promoting the construction of a standardized evaluation system and conducting cross-study comparisons through unified benchmark datasets and evaluation metrics, so as to fully unleash the technical potential of ML in efficient material design and precise regulation of chemical processes. Furthermore, the abbreviations used in this work are listed in Table 2.

Table 2. Abbreviation table.

Abbreviation	Full form	Abbreviation	Full form	Abbreviation	Full form
ACO	Ant Colony Optimization	JNU	Jinan University	TLBO	Teaching-Learning-Based Optimization
AIMD	Ab Initio Molecular Dynamics	KNN	K-Nearest Neighbor	VMD	Variational Mode Decomposition
ANN	Artificial Neural Network	LSTM	Long Short-Term Memory	VSA	Volume-Surface Area
AutoML	Automated Machine Learning	LSM	Least Squares Method	WGAN	Wasserstein Generative Adversarial Network
BNN	Bayesian Neural Network	LHS	Latin Hypercube Sampling	XAI	eXplainable Artificial Intelligence
Bi-RNN	Bidirectional Recurrent Neural Network	MAE	Mean Absolute Error	XGBoost	Extreme Gradient Boosting
BO	Bayesian Optimization	MAM	Metal Additive Manufacturing	YOLO	You Only Look Once
BRNN	Bidirectional Recurrent Neural Network	MBO	Multi-Objective Bayesian Optimization	XPS	X-Ray Photoelectron Spectroscopy
CA	Contact Angle	MB	Methylene Blue	XRD	X-Ray Diffraction
CFD	Computational Fluid Dynamics	ML	Machine Learning	MOFs	metal-organic frameworks
CGCNN	Crystal Graph Convolutional Neural Network	MLP	Multi-Layer Perceptron	ΔQ_{st}	Adsorption heat difference
CESVM	Cost-Effective Support Vector Machine	MLP	Multi-Layer Perceptron	S^0	Henry coefficient ratio
CGAN	Conditional Generative Adversarial Network	MOF	Metal-Organic Framework	PLD	Pore limiting diameter
CNN	Convolutional Neural Network	MR	Multiple Regression	LCD	largest cavity diameter
COPth	Coefficient of Performance (theoretical)	MSR	Molten Salt Reactor	GCD	global cavity diameter
CBM	Carbon-Based Material	NARX	Nonlinear AutoRegressive with eXogenous inputs	ASA	accessible surface area
CRAFT	Character-Region Awareness For Text detection	NLP	Natural Language Processing	V_F	void fraction
CV	Cross-Validation	NMSE	Normalized Mean Squared Error	SAH	Sodium Alginate-based Hydrogel
DCGAN	Deep Convolutional Generative Adversarial Network	NNP	Neural Network Potential	MB	Methylene Blue
DFT	Density Functional Theory	NRMSE	Normalized Root Mean Squared Error	DFT	Density Functional Theory
DT	Decision Tree	NO_3RR	Nitrate Electroreduction Reaction	ANN	Artificial Neural Network
DNN	Deep Neural Network	NNP	Neural Network Potential	Eads	Adsorption Energy
ECs	Emerging Contaminants	OC20	Open Catalyst 2020 Dataset	qe	Adsorption Capacity
Eads	Adsorption Energy	OER	Oxygen Evolution Reaction	RRMB	MB Removal Efficiency

Table 2. *Cont.*

Abbreviation	Full form	Abbreviation	Full form	Abbreviation	Full form
EIC	Electrical Insulation Conference	OL	Online Learning	EHOMO	Highest Occupied Molecular Orbital Energy
ERNN	Elman Recurrent Neural Network	PANN	Probabilistic Artificial Neural Network	ELUMO	Lowest Unoccupied Molecular Orbital Energy
ET	Extra Trees	PEOE	Partial Equalization of Orbital Electronegativity	Eg	Energy Gap
FE	Faradaic Efficiency	PID	Proportional Integral-Differential	χ	Electronegativity
FIIR	Fourier Transform Infrared Spectroscopy	PNN	Probabilistic Neural Network	η	Global Chemical Hardness
GAN	Generative Adversarial Network	RoBERTa	Robustly Optimized BERT Pretraining Approach	τb	breakthrough initiation time
GAT	Graph Attention Network	RPB	Rotating Packed Bed	Hi	Isosteric Heat of Adsorption
GBT	Gradient Boosting Tree	RSM	Response Surface Methodology	ΔUi,s	Adsorption Energy Parameter
GCMC	Grand Canonical Monte Carlo	SAR	Sodium Adsorption Ratio	mi,s	Saturation Adsorption Capacity Parameter
GCN	Graph Convolutional Network	SEM	Scanning Electron Microscopy	bi,s	Adsorption Affinity Parameter
GNN	Graph Neural Network	SHAP	Shapley Additive exPlanations	ρ_b	Adsorbent Particle Density
GPR	Gaussian Process Regression	SIP	Spectral Induced Polarization	C4.5	C4.5 Decision Tree Algorithm
GRNN	Generalized Regression Neural Network	SMX	Sulfamethoxazole	MAM	Metal Additive Manufacturing
GRU	Gated Recurrent Unit	SN	Signal-to-Noise Ratio	MAE	Mean Absolute Error
HDNNP	High-Dimensional Neural Network Potential	SMMs	Smart Manufacturing Systems	CTE	Coefficient of Thermal Expansion
HFC	Hydrofluorocarbon	SMILES	Simplified Molecular-Input Line-Entry System	NLP	Natural Language Processing
IAST	Ideal Adsorbed Solution Theory	SVM	Support Vector Machine	TGA	Thermogravimetric Analysis
ICANNGA	International Conference on Adaptive and Natural Computing Algorithms	SVR	Support Vector Regression	CIF	Crystallographic Information File
ICSP	International Conference on Signal Processing	TC	Tetracycline	RACs	Revised Autocorrelations
IPAS	International Conference on Image Processing Applications and Systems	Td	Decomposition Temperature	XRD	X-ray Diffraction
IR	Infrared	TEM	Transmission Electron Microscopy	MSR	Molten Salt Reactor
SEM	Scanning Electron Microscopy	TF	Term Frequency	CFD	Computational Fluid Dynamics
AIMD	Ab initio Molecular Dynamics	YOLO	You Only Look Once	MBO	Multi-objective Bayesian Optimization
IR	Infrared	CRAFT	Character-Region Awareness For Text detection	BRNN	Bayesian Regularization Neural Network
ACSF	Atom-Centered Symmetry Function	YOLO	You Only Look Once	RSM	Response Surface Methodology
HDNNP	High-Dimensional Neural Network Potential	COCO	Common Objects in Context	PSA	Pressure Swing Adsorption
OC20-Dense	Open Catalyst 2020-Dense Dataset	Mask R-CNN	Mask Region-based Convolutional Neural Network	DT	Digital Twin
SIP	Spectral Induced Polarization	FOM	Full-Order Model	LHS	Latin Hypercube Sampling
AC	Activated Carbon	POD	Proper Orthogonal Decomposition	MCMC	Markov Chain Monte Carlo
CV	Crystal Violet (cationic dye)	LSM	Least-Squares Method	DNN	Deep Neural Network
MO	Methyl Orange (anionic dye)	RF	Random Forest	NARX	Nonlinear Autoregressive with Exogenous Inputs
COPth	Thermal Coefficient of Performance	ET	Extra Trees	OL	Online Learning
ASO	Atom Search Optimization	ROM	Reduced-Order Model	STR	Stirred Tank Reactor
SCP	Specific Cooling Power	POD	Proper Orthogonal Decomposition	GPR	Gaussian Process Regression
CRN	Chemical Reactor Network	Bayeschem	Bayesian Theory of Chemisorption	DOS	Density of States
RANS	Reynolds-Averaged Navier–Stokes	NMR	Nuclear Magnetic Resonance	B2	Body-Centered Cubic Intermetallic Structure
FE	Faradaic Efficiency				

3. Machine learning models for different applications

Nonlinear processes play a pivotal role in numerous scientific research endeavors and engineering applications, particularly in the domains of chemical engineering, environmental engineering, and materials science. These complex processes typically entail nonlinear coupling relationships among multiple variables. Precisely predicting the behavior of nonlinear processes holds significant importance for optimizing design, enhancing efficiency, and minimizing costs. However, the complexity and challenge of nonlinear process modeling make the traditional method face many limitations in practical application. Traditional nonlinear process modeling methods usually rely on physical theoretical derivations, such as differential equations, statistical regression analysis, and the finite element method. These methods require researchers to first assume the form of the relationship between variables and then fit the model parameters using experimental data. However, in complex systems, the relationships between variables are often not linear and cannot be fully described by simple analytic expressions [50,51].

The rapid progress of artificial intelligence, especially the application of machine learning, has transformed nonlinear process prediction by providing substantial benefits in tackling complex problems without depending on explicit mathematical models. Among the diverse machine learning techniques, artificial neural networks (ANN) and support vector machines (SVM) are prominent as widely adopted models owing to their robust capabilities in nonlinear feature extraction, modeling, and prediction [52,53]. Inspired by biological neural networks, ANN has demonstrated exceptional proficiency in capturing complex nonlinear relationships across diverse fields, from network recommendation algorithms to astrophysics and industrial engineering, leveraging its powerful mapping and adaptive learning abilities. By utilizing multi-layer connections, it extracts deep features from data, constructing intricate models between input and output variables. On the other hand, SVM grounded in statistical learning theory, leverage kernel functions to transform non-linear challenges into high-dimensional feature spaces, facilitating the identification of optimal hyperplane [54]. As shows in Figure 1, nonlinear processes pose significant challenges in science and engineering, where traditional methods often fall short in modeling complex systems. ANN and SVM infuse this field with new vitality, efficiently capturing nonlinear relationships and facilitating system optimization and performance prediction. This chapter delves into these models, highlighting their transformative role in advancing nonlinear process research.

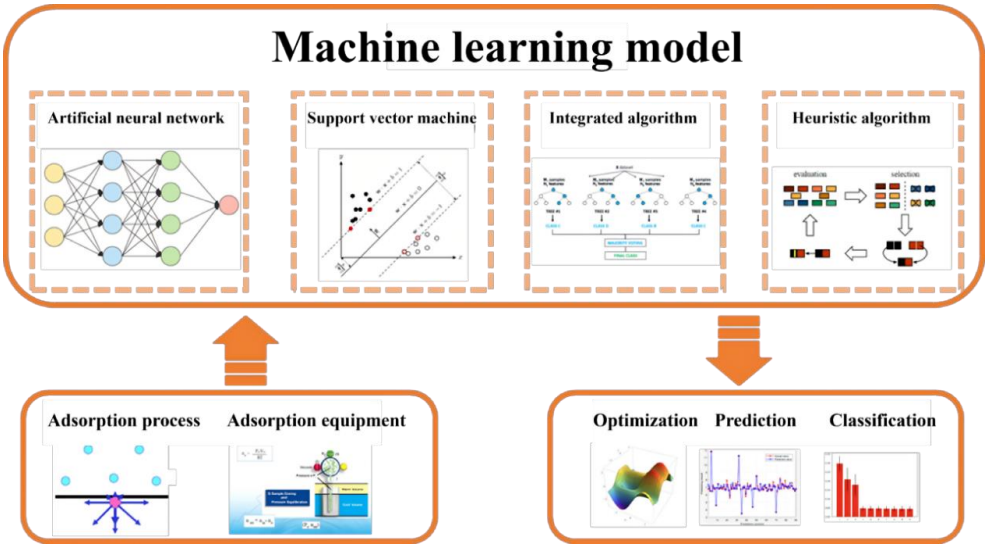

Figure 1. Application of machine learning model to adsorption.

3.1. Machine learning models for nonlinear process prediction

Nonlinear multivariate coupling is prevalent in adsorption systems, which limits the accuracy of traditional theoretical models. Machine learning provides powerful tools for nonlinear prediction without relying on explicit physical–chemical expressions. Artificial neural networks and support vector machines are widely used for their excellent capability in nonlinear feature extraction and prediction [55].

As illustrated in Figure 2a, the BP neural network receives input signals via forward propagation and updates network weights through backpropagation to minimize prediction errors [56,57]. As shown in Figure 2b, the RBF neural network maps low-dimensional data into a high-dimensional space to address linearly inseparable problems [58,59]. As depicted in Figure 2c, SVM constructs an optimal classification hyperplane and realizes linearization of nonlinear problems via kernel function mapping [60,61].

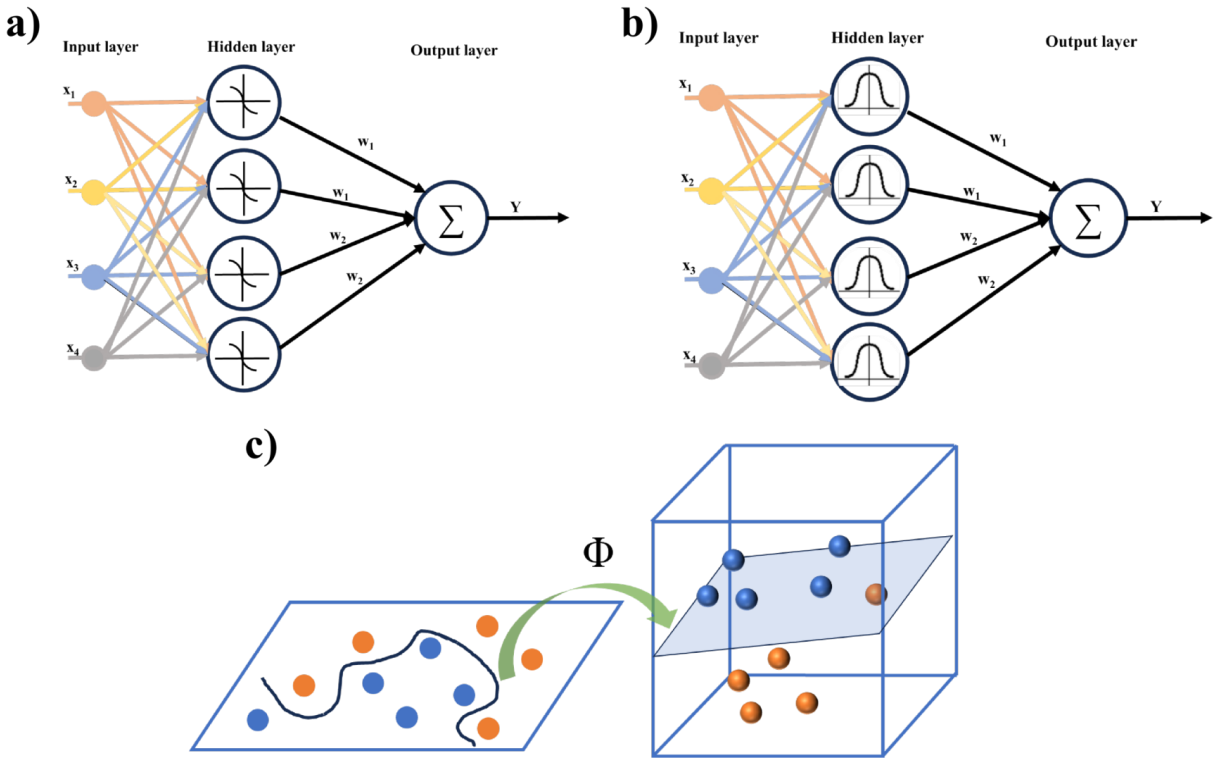

Figure 2. Schematic diagram of the model used in the field of nonlinear fitting: **(a)** BP neural network calculation process diagram; **(b)** RBF neural network calculation process diagram; **(c)** SVM classification principle schematic diagram.

In adsorption processes, the above models differ in their applicable scenarios. Artificial neural networks are suitable for handling the complex multivariate coupling relationships in adsorption processes and realizing information processing and pattern recognition. Specifically, BP neural networks are appropriate for scenarios requiring accurate prediction of adsorption performance and dynamic optimization of model parameters, whereas RBF neural networks are preferred when linearly inseparable multivariate problems exist in adsorption systems. Finally, support vector machines are suitable for classifying adsorption systems while ensuring strong generalization ability of the model.

3.2. Artificial neural networks for image applications

With the wide application of TEM, SEM, and *in-situ* imaging techniques, efficient image analysis has become increasingly important in adsorption research [62–64]. CNNs enable automatic, objective, and high-throughput feature extraction from microscopic images [65–68].

As shown in Figure 3a, CNNs extract image features through convolutional layers, compress data via pooling layers, and complete classification through fully connected layers [69,70]. As illustrated in Figure 3b, GNNs capture topological correlations in graph-structured data via node information aggregation, with typical models including GCN and GAT [71–73].

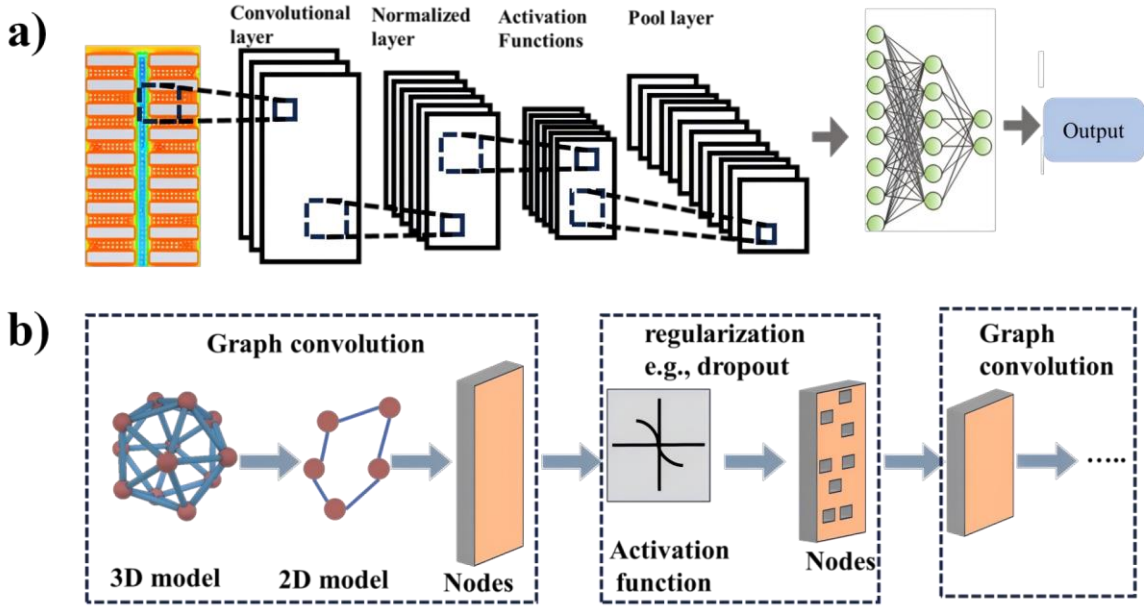

Figure 3. Schematic diagram of the model applied in the field of images: **(a)** Schematic diagram of convolutional neural network calculation process; **(b)** Schematic diagram of neural network calculation process.

When applied in the field of adsorption, convolutional neural networks are suitable for image analysis of adsorption systems. They can efficiently process characterization images such as TEM and SEM, accurately extract features including adsorbent morphology and adsorption sites, and assist in the monitoring and analysis of adsorption processes. Graph neural networks are applicable to scenarios with graph-structured characteristics in adsorption systems, which can capture information such as the molecular structure of adsorbents and the correlation of adsorption sites, thereby facilitating in-depth investigations into adsorption mechanisms.

3.3. Artificial neural networks for sequential data processing

Adsorption kinetics and dynamic processes are typical time-series problems. RNNs and Transformers represent mainstream approaches for sequential modeling [74–76]. As depicted in Figure 4a, RNNs capture short-term temporal dependencies through cyclic network connections. Variants such as LSTM solve the vanishing gradient problem using gating mechanisms [77–80]. As shown in Figure 4b, Transformers rely on multi-head self-attention and positional encoding, enabling parallel processing and superior performance in long time-series data [81,82].

For problems concerning adsorption processes, recurrent neural networks and their variants are suitable for modeling short-term sequential adsorption data. They can accurately capture the short-term dependencies of adsorption rate and adsorption capacity as functions of time, making them ideal for the prediction of adsorption kinetic processes. Transformers are applicable to the processing of long-term sequential adsorption data, capable of capturing the long-term coupled dynamic relationships among multiple factors during adsorption, and thus suitable for long-term prediction and dynamic behavior analysis of complex adsorption systems.

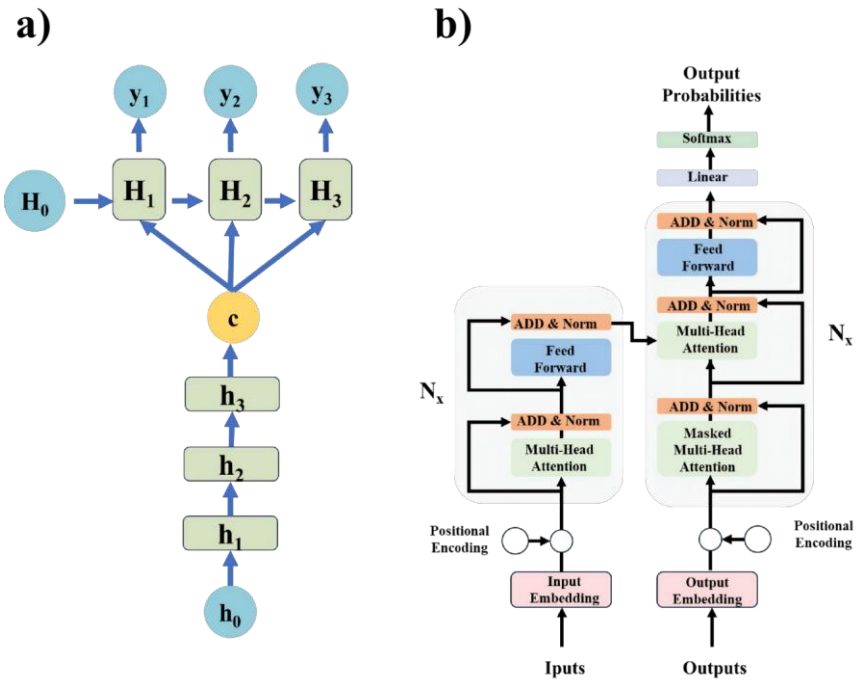

Figure 4. Schematic diagram of the model for sequential data processing: **(a)** Recurrent neural network calculation diagram; **(b)** Transformer neural network calculation diagram.

3.4. Neural networks for generative tasks

Generative artificial intelligence exhibits broad application potential in the fields of chemical process optimization, molecular design, and material design [83,84]. Traditional chemical optimization methods based on mathematical modeling struggle to capture the global characteristics of complex systems, whereas generative models can learn from historical data to generate optimized operating conditions or reaction pathways, and can be combined with reinforcement learning to achieve intelligent control [85,86].

GANs were proposed by Ian Goodfellow *et al.* in 2014. Their core framework adopts an adversarial game between two modules: a generator and a discriminator [87,88]. The generator produces synthetic data, while the discriminator distinguishes between real and synthetic data. The two components are trained alternately and mutually optimized in an unsupervised learning manner without requiring labeled data [89,90]. Its variants, such as CGAN, DCGAN, and WGAN, improve the framework by refining loss functions and introducing additional constraints [91,92]. GANs and other generative models have promoted the transformation of research in chemical engineering from experiment-driven to data-driven paradigms.

GANs are suitable for scenarios including adsorption condition optimization, adsorbent molecular design, and adsorption reaction pathway planning. By learning from historical adsorption data, they can

generate optimal adsorption operating parameters, novel high-efficiency adsorbent molecular structures, and feasible adsorption reaction pathways, laying a foundation for the intelligent optimization of adsorption processes.

3.5. Algorithms for optimization

Heuristic algorithms mainly include GA, PSO, and ACO. These algorithms feature high flexibility and adaptability, and excel in solving nonlinear and multimodal problems [93]. Each algorithm has its own framework with distinct characteristics.

As illustrated in Figure 5a the framework of Genetic Algorithm is rooted in biological evolutionary theory. It conducts iterative optimization through a four-step cycle: encoding, selection, crossover, and mutation, simulating natural selection to optimize adsorption and separation conditions [94,95]. In addition, as shown in Figure 5b, the Particle Swarm Optimization framework mimics the foraging behavior of birds, rapidly searching for optimal solutions by updating individual positions and sharing global optimal information [96]. The Ant Colony Optimization framework simulates the path-finding behavior of ants during foraging, guiding the search process via pheromone concentration variations to optimize multicomponent adsorption and separation pathways [97,98].

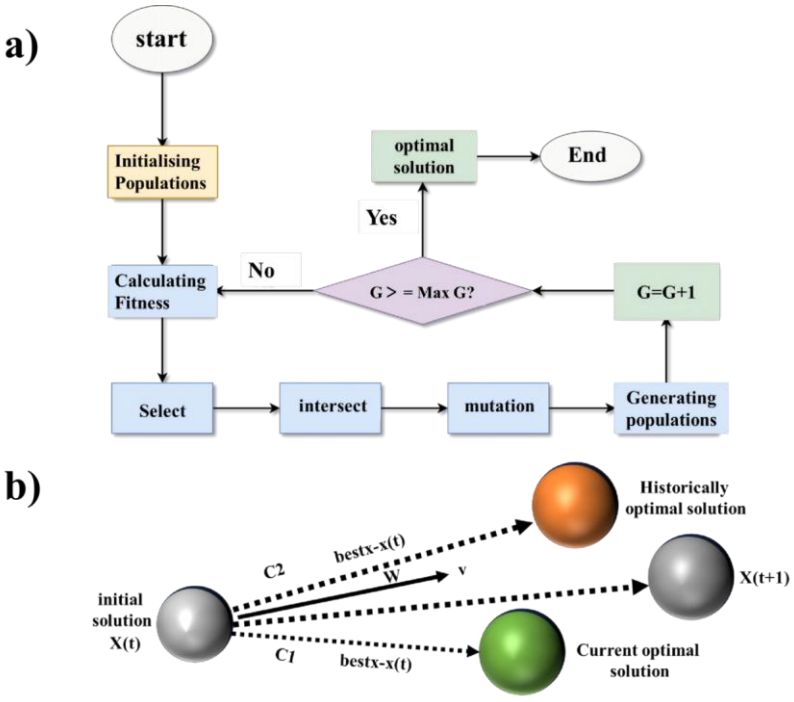

Figure 5. Model schematic for the field of single-objective optimization: **(a)** genetic algorithm; **(b)** particle swarm optimization.

Heuristic algorithms originated in the mid-1950s and follow a neighborhood search procedure, which can be categorized into single-objective optimization and multi-objective optimization [99,100]. Single-objective optimization includes Genetic Algorithm, systematically formulated in 1975 [101,102], and Particle Swarm Optimization, proposed in 1995 [103,104]. Multi-objective optimization relies on the Pareto front. As illustrated in Figure 6, the ensemble learning framework introduced in 1979 is centered on performance improvement via multi-model fusion, covering stacking(Figure 6a), bagging (Figure 6b), and boosting algorithms [105–107].

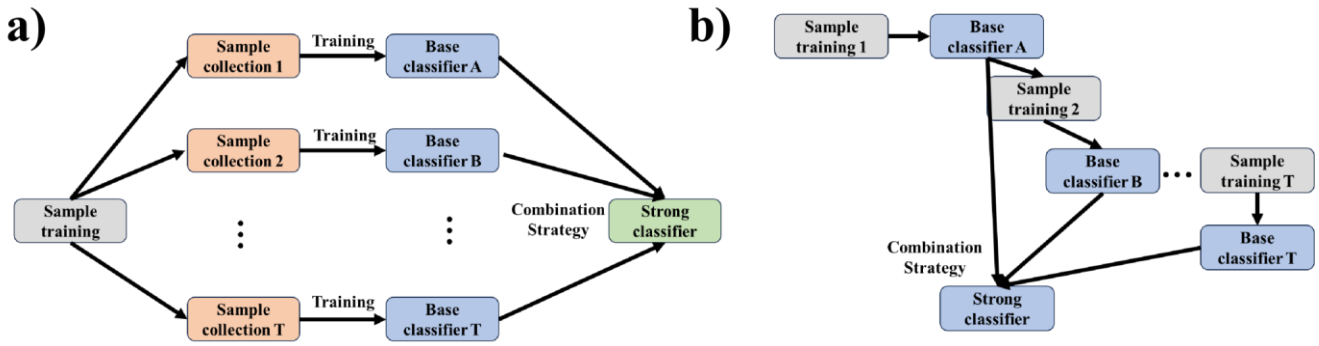

Figure 6. Model schematic for the field of multi-objective optimization: **(a)** Calculation diagram of Stacking algorithm; **(b)** bagging algorithm calculation diagram.

In adsorption applications, genetic algorithms are suitable for optimizing multivariate nonlinear adsorption conditions and can efficiently determine the optimal combination of adsorption parameters. Particle swarm optimization is applicable to the dynamic optimization of adsorption processes, enabling rapid adaptation to dynamic variations in adsorption systems and searching for approximate global optimal adsorption conditions. Ant colony optimization is suitable for optimizing separation pathways in multicomponent adsorption. Ensemble learning is ideal for high-precision prediction of adsorption performance, improving the accuracy and stability of adsorption predictions via multi-model fusion.

3.6. Other machine learning models

Bayesian models were proposed in the 18th century by Thomas Bayes. As illustrated in Figure 7, the core framework is based on Bayes' theorem, which addresses uncertainty problems by integrating prior knowledge and observed data through the derivation of prior probability, likelihood probability, and posterior probability, showing excellent performance on small-scale datasets [108,109]. The Naive Bayes model is established on the basis of Bayes' theorem and the conditional independence assumption of features, which simplifies the computational procedure. Its derived models have been widely used in text classification, spam filtering, and other related fields [110,111].

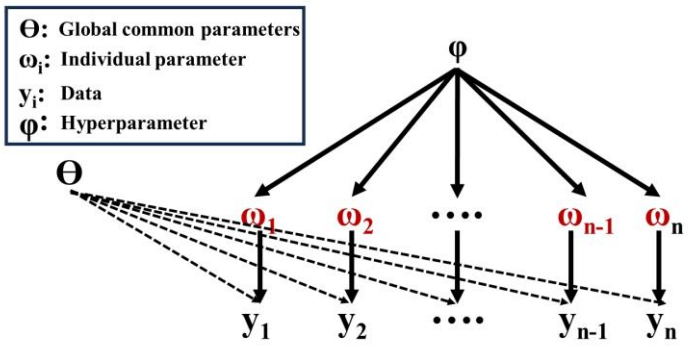

Figure 7. Hierarchical Bayesian model.

Machine learning potential models originated from the early neural network potential (NNP). Their core framework lies in data-driven modeling instead of traditional theoretical modeling, which can replace costly conventional potential functions with higher prediction accuracy and computational efficiency. These models establish predictive frameworks by learning the rules of atomic interactions. The

derived deep potential models further optimize the construction of potential energy surfaces through deep networks and have been widely employed in molecular simulations within materials science [112,113].

3.7. Relationship between machine learning models and adsorption processes

Traditional adsorption models reveal fundamental mechanisms but rely on simplified assumptions. Machine learning models serve as a powerful complement by handling high-dimensional, nonlinear, and strongly coupled adsorption systems.Linear models provide high interpretability and act as baseline benchmarks. Tree-based ensemble models efficiently capture nonlinear correlations. Neural networks support complex mechanism simulation, image analysis, time-series prediction, and intelligent adsorbent design.

In summary, traditional theoretical models are essential for understanding adsorption fundamentals, whereas machine learning models excel at high-precision prediction, multi-factor optimization, and data-driven discovery. The combination of theoretical analysis and machine learning will strongly promote the development of adsorption science and engineering.

4. Application of machine learning in adsorption field

4.1. Design and research of machine learning-assisted adsorbent

As the core of the adsorption process, the design of adsorption materials plays a crucial role in the adsorption process. Conventionally, the development of adsorbent materials has relied on continuous iterative experimentation and the “chemical intuition” of chemists. Although this approach has achieved a certain degree of success, it also encounters numerous challenges and limitations. In this context, the emergence of machine learning offers novel perspectives and tools for the design and development of adsorbent materials [114]. As a significant branch of artificial intelligence, machine learning excels at processing complex data sets and extracting valuable information from them. Its core advantage lies in its capacity to establish accurate models and predictions for non-linear processes. By analyzing extensive experimental data and relevant literature, machine learning can assist researchers in identifying underlying patterns and relationships, providing a scientific foundation for the material development process. This data-driven approach not only enhances the efficiency of material design but also reduces the uncertainty in the development process. In this chapter, the design of machine-learning-assisted adsorbents is divided into the following sections: (1) Design and development of adsorbents; (2) High-throughput screening of adsorbents; (3) Characterization and evaluation of adsorbents.

4.1.1. Novel high-throughput screening strategies for adsorbents

The high-throughput screening strategy mainly involves using machine learning to discover the intrinsic relationships between data, and then conducting a preliminary screening of the performance of adsorption materials. However, the biggest limitation of machine learning and the adsorption process lies in how to describe the complex adsorption process. Current research has shown that by using theoretical calculation methods to obtain the most closely related descriptors to the adsorption process, and using these descriptors as intermediate variables to input the complex adsorption process into the machine learning model. As shown in Figure 8a, Li *et al.* based on the random forest algorithm explored the relative importance of structural and energy descriptors and the correlation between the propane/propane selectivity of these MOFs and their descriptors. Through detailed data analysis, the

author proposed that first using structural descriptors to conduct a preliminary screening of the MOF structure, and then using energy descriptors to further confirm the MOF structure with high propane/propane selectivity, can save a large amount of computing resources [19]. Furthermore, some studies have adopted a combined approach of using machine learning, density functional theory, and other methods to establish the functional relationship between the performance and structural parameters of adsorbents, in order to predict the performance of adsorbent materials and screen for adsorbents. For example, as shown in Figure 8b, by combining DFT calculations with machine learning tools, the sodium alginate hydrogel adsorbent was optimized to effectively adsorb water pollutants. Compared to energy descriptors, this method enables the optimization and preparation of adsorbent materials [20].

During the adsorption process, aside from the design of the adsorption material, another core aspect is the exploration of the adsorption process. Nevertheless, due to the nonlinear nature of the multi-component adsorption process, it is arduous to model multi-component adsorption using conventional methods. Consequently, machine learning can aid in formulating nonlinear models for multi-component adsorption processes.The earliest research that employed machine learning for nonlinear modeling aimed to predict the adsorption process of multiple components via artificial neural networks, as depicted in Figure 8c. Su *et al.* adopted artificial neural networks as a novel computational approach and initially applied it to the modeling of seven multi-component adsorption systems [21]. This study successfully utilized a backpropagation neural network model with saturation transfer functions. The results demonstrated that the adsorption isotherms generated by the artificial neural network model exhibited a significantly superior correlation with the experimental data compared to the outcomes of the multi-component Langmuir model.

Although this research pioneered the application of artificial neural networks in the field of adsorption processes, due to the constraints of computing conditions at that time, the research on artificial neural networks gradually fell behind. It was not until the development of the computer industry in recent years that the integration of artificial neural networks and adsorption processes gradually became more intimate. As shown in Figure 8d, Arora *et al.* developed a method grounded in artificial neural networks for the efficient screening of microporous materials suitable for gas separation. This method can rapidly predict the transient adsorption behavior and breakthrough time of the materials while preserving the accuracy of the prediction. Moreover, this research introduced the concept of breakthrough event time and constructed an artificial neural network model to precisely predict these times. This method can assess the performance of different materials in terms of column breakthrough time [22].

It can be observed that with the enhancement of computing power, this artificial neural network model based on nonlinear processes has gradually become applicable to process research. However, the interpretability of artificial neural networks remains a crucial limitation for their application in the field of adsorption.

Artificial neural networks, characterized by their potent nonlinear fitting capabilities, outstanding generalization performance, and robustness, have emerged as an optimal instrument for addressing intricate nonlinear issues in the adsorption process. Nevertheless, artificial neural networks also exhibit certain limitations, including a complex training procedure, poor interpretability, and a propensity for overfitting. These challenges render it arduous for artificial neural networks to manage the adsorption process with small-sample characteristics, and the “black-box” feature makes it difficult for them to precisely depict the adsorption process. Consequently, enhancing the interpretability of the artificial neural

network model, reducing its dependence on a substantial amount of labeled data, and strengthening the model's generalization ability to prevent overfitting are the cruxes of the application of artificial neural networks in the adsorption domain.

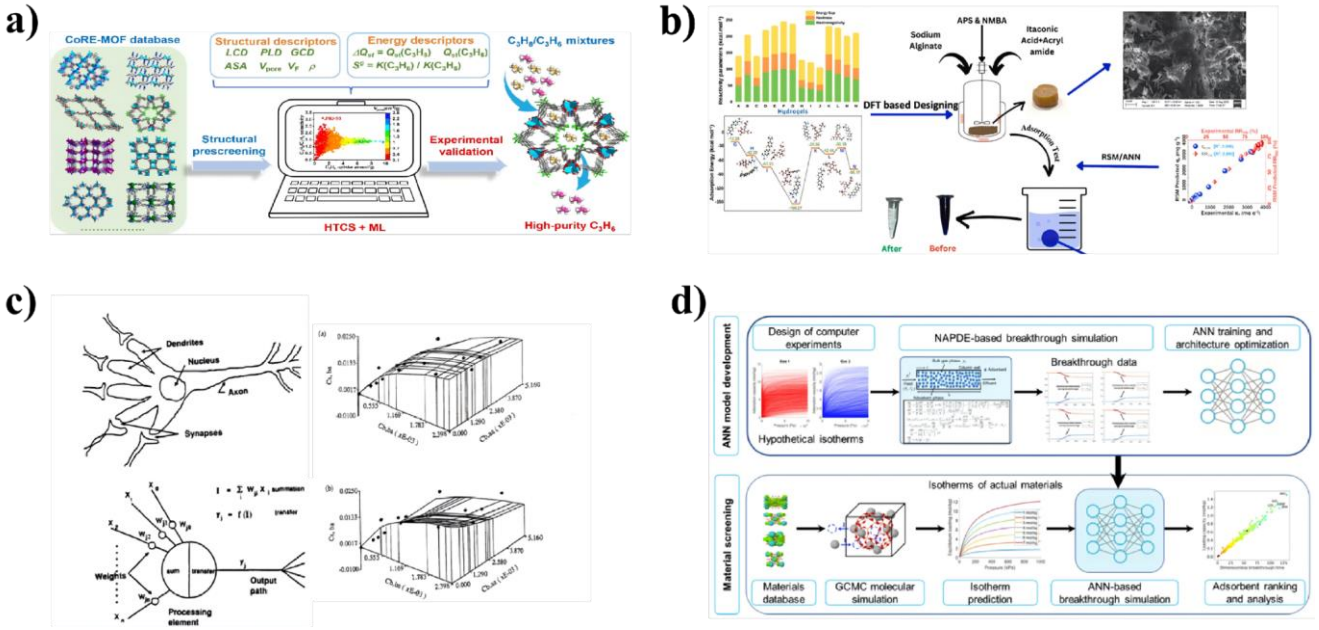

Figure 8. Research related to high-throughput screening strategies for adsorbents: **(a)** Using random forests to explore and screen the MOF structure [19]. Reprinted with permission. Copyright 2024 ACS; **(b)** Optimization of sodium alginate using machine learning combined with DFT [20]. Reprinted with permission. Copyright 2024 Elsevier; **(c)** Artificial neural networks are used for modeling multi-component adsorption [21]. Reprinted with permission. Copyright 1993 Springer Nature; **(d)** Artificial neural network for high-throughput material screening [22]. Reprinted with permission. Copyright 2020 ACS.

4.1.2. New design strategy for adsorption materials

The traditional design method of adsorbent materials is a complex and delicate process, which mainly relies on literature research, material science principles and many empirical attempts. This approach requires researchers to have not only a wealth of chemical knowledge, but also a deep understanding and practical experience of the adsorption process and material properties to achieve efficient design of adsorbed materials. However, with the continuous progress of material science and the development of science and technology, the structure of new materials is becoming increasingly complex, and traditional design theories and methods are gradually difficult to meet these challenges. This complexity is not only reflected in the chemical composition and structure of the material, but also in its stability and adsorption properties under different temperature, pressure and chemical environments. In the face of these new challenges, it is difficult to make breakthroughs in a short time. The rapid development of machine learning provides a new solution for adsorption material design. By using machine learning techniques, a complex correlation model between the properties of adsorbed materials and their structural parameters can be established. These models are able to learn the behavior patterns of adsorbed materials from large amounts of data and provide fast and accurate performance predictions without the need for extensive experiments.

This chemical informatics approach facilitates the input of material data into machine learning models, and the adsorption process is grounded in empirical research. Consequently, integrating the accumulated process knowledge into the machine learning model to construct a semi-interpretable model has emerged as a research focus. For example, as shown in Figure 9a, Paul *et al.* explored how to utilize machine learning algorithms to predict the outcomes of chemical reactions. This research collected data from failed or unsuccessful hydrothermal synthesis experiments in laboratory notebooks, and combined with chemical informatics techniques to add physical and chemical attribute descriptions to the original data. Using these data, the research trained a machine learning model to predict the success rate of material synthesis. Moreover, by using the machine learning model in reverse, the author proposed new hypotheses regarding the conditions required for the successful formation of products [115]. Although this chemical informatics approach enables the input of material data into machine learning models, the adsorption process is based on empirical research. Therefore, adding the accumulated process knowledge to the machine learning model to form a semi-explainable model has become a research hotspot. As depicted in Figure 9b, Aftab *et al.* employed an [23] empirical-based support vector regression (SVR) to forecast the adsorption of phenol by activated carbon in a rotating packed bed. The findings demonstrated that the accuracy of the SVR results was comparable to those predicted by the ANN, yet the SVR exhibited superior interpretability relative to the ANN.

Beyond ANN and SVR, the random forest algorithm can also be utilized for regression prediction in the adsorption process. As shown in Figure 9c, Zhu *et al.* applied machine learning to develop a general prediction model for the adsorption of tetracycline and sulfamethoxazole (SMX) on carbon-based materials. This research indicated that for the adsorption models of TC and SMX, the random forest outperformed the gradient boosting tree and artificial neural network [24].

Most of the aforementioned approaches strive to enhance the interpretability of the model via information science or the integration of empirical knowledge. This methodology can be applied to materials or process studies characterized by small data volumes and well-defined processes. However, for adsorption processes featuring large data volumes and unclear research processes, another study employed machine learning to analyze the significance of the data and conducted research on the adsorption process. Random forest, as a crucial novel analytical model, is extensively utilized in this domain. As depicted in Figure 9d, Zeeshan's research forecasted the adsorption capacity of biochar materials for emerging pollutants (ECs) in water by establishing a tree-based machine learning model. The study compared 10 ML models and discovered that CatBoost was the most effective in predicting adsorption capacity, with the highest coefficient of test determination and the lowest mean absolute error. SHAP analysis indicated that the adsorption experimental conditions exerted the greatest influence on the prediction of the adsorption capacity model, followed by the adsorbent composition, characterization, and synthesis conditions [25].

Currently, algorithms with a certain degree of interpretability, such as random forests, are primarily employed for material design. However, in comparison with other machine learning models, the most prominent characteristic of random forests is that they offer a measure of feature importance, which is beneficial for feature selection and data comprehension. Nevertheless, random forests encounter issues such as prolonged training time and high memory requirements. In the future, the development direction of random forests should concentrate on enhancing the interpretability of the model, reducing the risk of overfitting, and optimizing the algorithm to decrease memory usage.

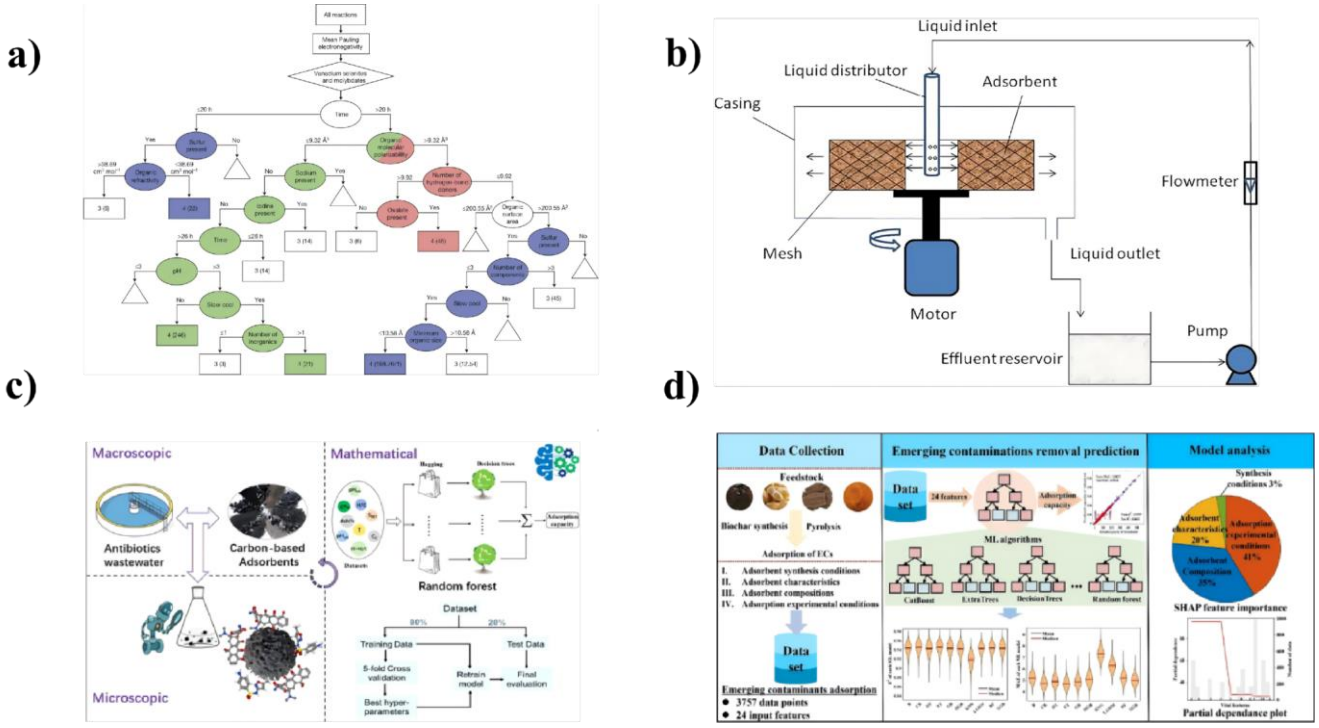

Figure 9. Research on the Application of Machine Learning in Designing Instructional Materials: **(a)** Classification principle of support vector machine [115]. Reprinted with permission. Copyright 2016 Springer Nature; **(b)** Support vector machines are used to predict chemical reactions [23]. Reprinted with permission. Copyright 2023 Springer Nature; **(c)** Using machine learning to explore the importance of carbon-based materials [24]. Reprinted with permission. Copyright 2021 Elsevier; **(d)** Using random forest to predict the adsorption performance of carbon materials for pollutants [25]. Reprinted with permission. Copyright 2023 Elsevier.

4.1.3. Characterization and evaluation of adsorbents

In the realm of adsorbent materials, the characterization and analysis of materials represent critical stages. Conventional material characterization methods typically depend on diverse experimental techniques to acquire the micro-structure, composition, and morphology of materials. Nevertheless, the collection of such data merely constitutes the initial phase of material characterization. Subsequently, the interpretation and analysis of images and data frequently rely on the expertise and subjective discernment of the researcher. This manual analytical approach is not only time-consuming but also highly susceptible to human factors, potentially leading to biases and inconsistencies in data interpretation.When confronted with intricate material structures and extensive volumes of characterization data, the limitations of this traditional approach become increasingly prominent. Simultaneously, with the rapid advancement of materials science, researchers' comprehension of the depth and breadth of material structure and properties is continuously expanding. Traditional characterization methods struggle to meet the requirements of contemporary materials research. Against this backdrop, machine learning technology offers a novel strategy and methodology for the characterization and analysis of adsorbent materials. It significantly enhances the efficiency and accuracy of characterization through automated and intelligent data processing and analysis. Machine learning excels at discerning complex patterns and relationships from vast amounts of data, a

characteristic that demonstrates substantial potential in the processing and analysis of material characterization data.

Particularly in the domain of image analysis, deep learning algorithms within machine learning, such as CNN, can automatically extract features from representative images and conduct classification and recognition. These algorithms possess significant advantages over traditional manual analysis methods. Through training, these algorithms can identify and quantify key features such as micro-structure and defects in material images, yielding more objective and consistent results compared to manual analysis.

The prevalent material characterization methods primarily involve identifying representative images via convolutional neural networks, establishing the nonlinear relationship between these representative images and material properties, and subsequently guiding the characterization design of materials. As depicted in Figure 10a, Akbari *et al.* constructed a machine-learning model to forecast mechanical properties, including yield strength, tensile strength, elastic modulus, elongation, hardness, and surface roughness, by analyzing machining parameters and material properties. The microstructure features in electron microscope images are correlated with the impact energy in mechanical tests to predict the mechanical properties of materials [26]. Machine learning not only has the capability to predict readily measurable data but also offers the significant advantage of predicting certain data that are challenging to measure. For instance, Nandy *et al.* provided a machine-learning model with 3000 MOFs stability data. These models can be employed to predict the solvent removal stability and thermal stability of MOFs, which is crucial for evaluating the mechanical properties and stability of adsorbents [27].

The most significant issue in machine learning pertains to the acquisition of data samples. Consequently, how to acquire a substantial volume of effective data has emerged as a challenge that constrains the application of machine learning in representation prediction. Through the integration of representations, it has become a strategy for augmenting the learning samples of machine learning models. This approach facilitates the quantitative analysis of intricate processes. For instance, as shown in Figure 10b, as Jin *et al.* reported a straightforward and expeditious protocol founded on deep-learning technology, which is employed to address the complex phase identification and quantification problems in complex multiphase inorganic compounds. This research simulated the powder X-ray diffraction (XRD) spectra of 170 Sr-Li-Al-O four-component composition pools of inorganic compounds. Ultimately, the simulated powder XRD spectra of 170 inorganic compounds were combined and blended to obtain a large quantity of XRD spectra. A convolutional neural network (CNN) model was constructed, and the prepared substantial amount of data was utilized for the final training. The fully trained CNN model can promptly and precisely identify the components and phases of complex heterogeneous inorganic compounds [28].

Machine learning techniques are utilized to quantitatively extract particle size, particle size distribution, and morphological information from scanning electron microscopy (SEM) images. As shown in Figure 10c, this approach enables automated and high-throughput measurements, even when dealing with overlapping nanoparticles, rod-like structures, and core-shell nanostructures [29].

Machine learning not only optimizes the representation methods for images, such as SEM, but also has the potential to optimize spectroscopic characterization methods, like infrared spectroscopy. As depicted in Figure10d, Michael Gastegger *et al.* applied machine learning to predict highly accurate molecular infrared spectra. This research adopted a machine learning strategy to conduct ab initio molecular dynamics simulations, thereby accounting for the non-harmonicity of vibrations and dynamic effects. Through the application of machine learning, this study notably reduced the computational

burden in the theoretical calculation process. This work can yield highly accurate machine learning models based on several hundred electronic structure reference points, which can be employed for the prediction of infrared spectra [30].

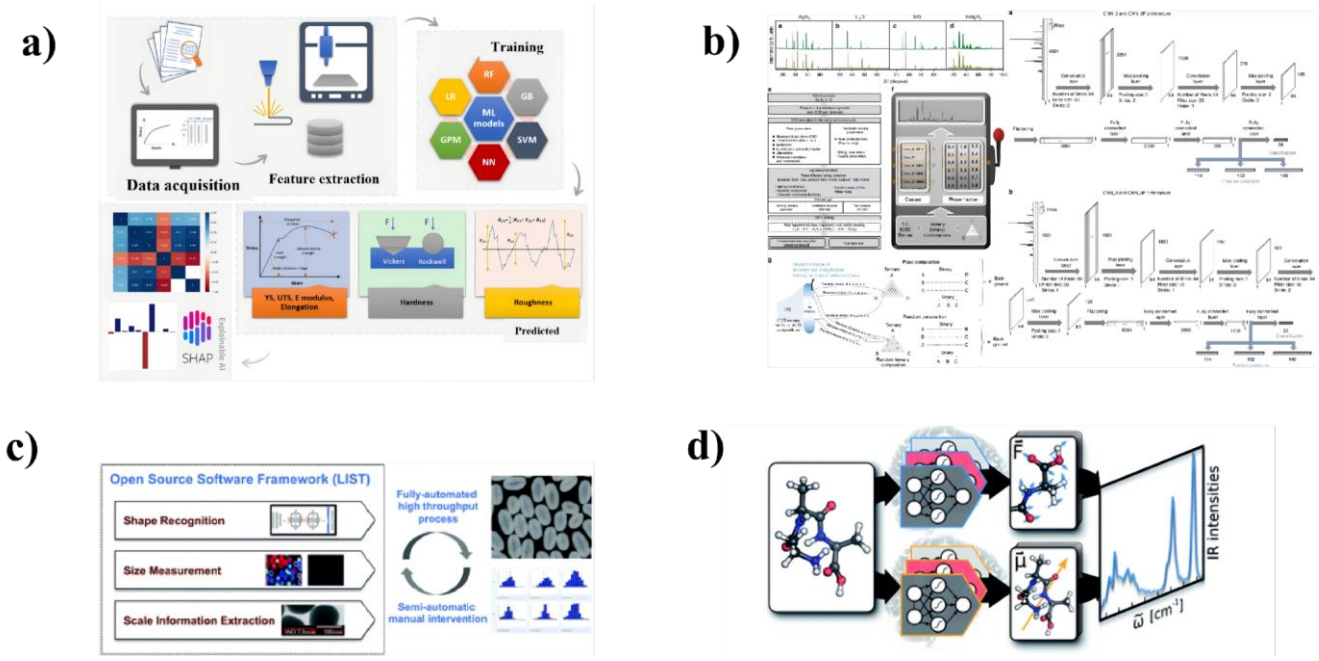

Figure 10. Research on the characterization and evaluation of adsorbents guided by machine learning: **(a)** Prediction of mechanical properties of machine learning-aided materials [26]. Reprinted with permission. Copyright 2024 Elsevier; **(b)** Machine learning combined with XRD [28]. Reprinted with permission. Copyright 2022 Springer Nature; **(c)** Machine learning combined with SEM [29]. Reprinted with permission. Copyright 2020 Springer Nature; **(d)** Machine learning combined with infrared [30]. Reprinted with permission. Copyright 2020 The Royal Society of Chemistry.

The application of machine learning in the field of adsorbent design and research has brought about methodological innovations, shifting from the traditional trial-and-error approach to data-driven rational design. This has significantly improved the efficiency of research and development and reduced uncertainty. Especially in handling nonlinear complex problems such as multi-component adsorption, it demonstrates strong capabilities. At the same time, it has achieved automation and intelligence in high-throughput screening and material characterization, reducing human errors. However, current applications still face many challenges. Firstly, models such as artificial neural networks have the “black box” problem, lacking interpretability, making it difficult to reveal the physical and chemical essence, and the model performance is highly dependent on high-quality and large-scale labeled data, while the acquisition of relevant data is costly. Secondly, in practical applications, the complexity of model selection, the importance of feature engineering, and the quality and standardization of representation data also urgently need to be addressed. Future research should focus on improving the interpretability of models, developing hybrid intelligent models that integrate physical and chemical principles, and strengthening the integration of multiple scales and multiple physical fields to construct predictive models from the microscopic to the macroscopic level.

4.2. Research on machine learning-assisted adsorption process

4.2.1. Optimization of multi-component adsorption process

The adsorption process typically encompasses multi-component systems, as most actual working conditions inevitably contain impurities. Nevertheless, traditional adsorption research and model construction predominantly concentrate on single-component systems. Traditional methods often prove inadequate for multi-component adsorption, particularly in dealing with complex interaction and competitive adsorption phenomena. The underlying cause is that traditional multi-component adsorption models are generally constructed based on experimental data and rely on fundamental assumptions regarding the interaction of components within the system and simplified treatments of the actual process. Such models exhibit limited ability to analyze the strong interaction between components or the competition for adsorption sites.

Likewise, machine learning, with its robust data-processing capabilities and pattern-recognition capabilities, offers an entirely novel approach to modeling and predicting multi-component adsorption processes. These models are no longer restricted to the modeling analysis of a single component but can concurrently consider the dynamic behavior and interaction of multiple components during the adsorption process. Moreover, machine learning models possess high adaptability and extensibility and can be updated and optimized based on new experimental data to continuously enhance their predictive performance.

The optimization of the multi-component adsorption process using machine learning primarily involves leveraging machine learning to assist in multi-component nonlinear modeling and explore multi-component interactions. There are relatively few comparable studies.

4.2.2. Prediction of adsorption process parameters

The essence of the adsorption process is a highly intricate nonlinear process that encompasses the interplay of numerous physicochemical mechanisms. Consequently, numerous parameters of the adsorption process are arduous to measure via conventional approaches and can only be acquired through the fitting of the adsorption process model. Traditional methodologies frequently rely on the fitting of kinetic and thermodynamic models for indirect prediction. Traditional parameter determination methods typically hinge on the fitting of classical kinetic models and thermodynamic models. The kinetic and thermodynamic constants are computed by matching experimental data with the model. Although these methods can offer valid estimations in certain instances, their application is often constrained by experimental conditions, data quality, and model assumptions. Confronted with these challenges, the advancement of machine learning technology presents a novel concept and method for the determination and prediction of adsorption process parameters. Through its potent data modeling and pattern recognition capabilities, machine learning can effectively handle the nonlinear relationships and complex and variable data characteristics in the adsorption process and attain rapid and precise prediction of key parameters.

The prevalent approach for parameter prediction in the adsorption process primarily involves utilizing machine learning models to construct models for the nonlinear process, thereby attaining precise prediction of nonlinear processes. As depicted in Figure 11a, Liu *et al.* developed a machine-learning model, trained AI to extract the structural parameters of porous materials for the prediction of water adsorption isotherms, and further estimated the cooling performance of various adsorbents and subsequent

applications based on this. In this research, the random forest model is employed to accurately predict the water adsorption isotherm of porous materials beyond the database, and it can distinguish the structural differences of materials to a certain degree [116]. Furthermore, as depicted in Figure 11b, Lyu *et al.* employed machine-learning techniques to simulate and forecast the performance of biochar serving as a phosphorus-removal adsorbent. The Random Forest (RF) and CatBoost algorithms were utilized to construct a predictive model through meticulous adjustment of crucial hyperparameters. This research offers in-depth understandings of the factors influencing the efficiency of phosphorus removal and furnishes guidance for the functionalization of biochar and the optimization of operating conditions [117]. The adsorption process can be modeled via machine learning, and the unknown parameters can be predicted in this manner. As depicted in Figure 11c, Zhu *et al.* constructed a model utilizing random forest to forecast the adsorption of tetracycline and Sulfamethoxazole on carbon-based materials (CBM). This model is capable of precisely predicting the adsorption quantity of antibiotics on carbon-based materials and demonstrates that its generalization ability under different environmental conditions and across various types of adsorbents surpasses that of the traditional isothermal model. Through relative importance analysis and partial dependence analysis, it was discovered that the specific surface area is of critical importance for the adsorption of tetracycline and sulfamethoxazole, whereas the influence of other material properties varies according to the molecular structure and functional groups of the antibiotics [31]. Therefore, in the prediction of chemical processes, machine learning is mainly reflected in the high-precision prediction of processes that are difficult to measure in the middle, thereby enhancing the understanding of complex chemical processes.

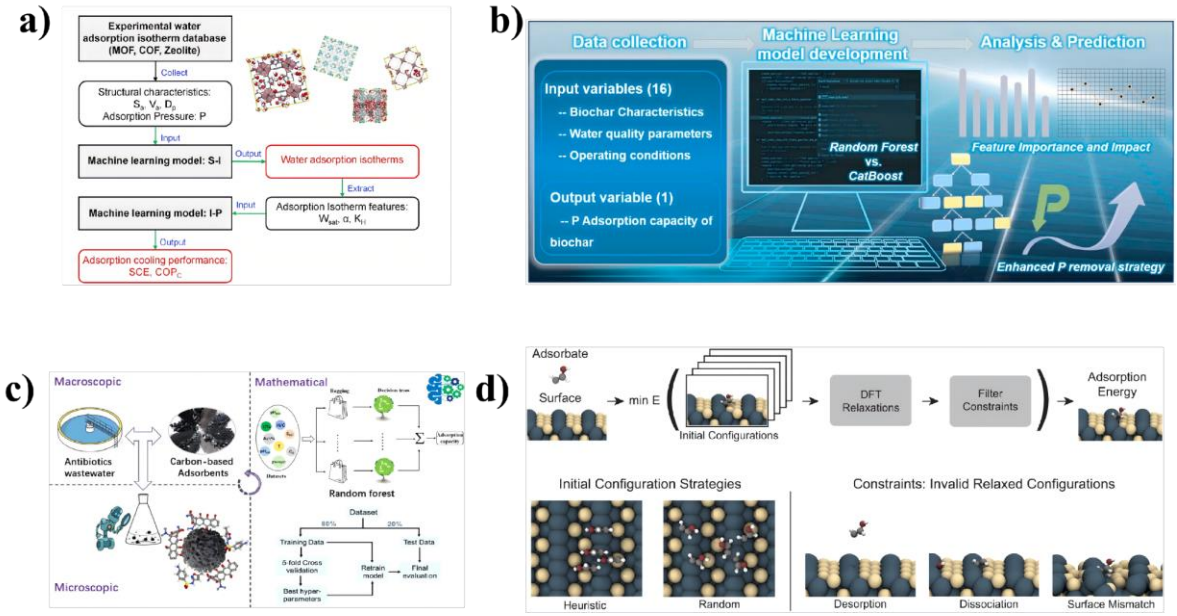

Figure 11. Research on machine learning for predicting parameters of adsorption processes: **(a)** The water absorption isotherm of porous material was predicted by random forest [116]. Reprinted with permission. Copyright 2024 The Royal Society of Chemistry; **(b)** The utilization of random forests for the functionalization of biochar and optimization of operating conditions [117]. Reprinted with permission. Copyright 2024 The Royal Society of Chemistry; **(c)** Using random forest to predict the absorbability of CBM [31]. Reprinted with permission. Copyright 2023 Springer Nature; **(d)** Machine learning potential energy is used to identify the surface structure of low energy adsorbent [32]. Reprinted with permission. Copyright 2022 Elsevier.

In addition, there are studies that employ machine-learning potential energy to explore unpredictable adsorption energy. As depicted in Figure 11d, Lan *et al.* put forward an algorithm named "AdsorbML", which makes use of a general machine-learning potential energy to expedite the calculation of adsorption energy. AdsorbML locates the lowest-energy configuration and attains a balance between accuracy and efficiency via various trade-offs. This suggests that machine learning can be utilized to more precisely and efficiently identify lower-energy adsorben-urface configurations [32].

Although the prediction of position parameters in the adsorption process can be realized through machine learning, the training process of machine learning models demands a substantial amount of data. This poses challenges in training machine learning models for numerous data that are difficult to acquire in the adsorption process, such as the mass transfer adsorption rate constant and the bed saturation adsorption capacity. Therefore, with the future development of small-sample models, the prediction process for such hard-to-obtain data will also be resolved.

4.2.3. Adsorption process monitoring and control

Owing to its rapid and transient attributes, the adsorption process has emerged as a crucial component of practical operations. The key lies in how to achieve precise regulation of the adsorption process to enhance production efficiency and product quality. Traditional control methods predominantly rely on proportional integral-differential (PID) control. Due to its simplicity and ease of implementation, PID control has been extensively applied in the industrial domain. PID control can adjust the system's output through proportional, integral, and differential operations on the error signal, thereby attaining the desired control effect.

Nevertheless, PID control often proves insufficient when addressing the rapid changes and transient characteristics of the adsorption process. The underlying reason is that PID control is founded on linear control theory, whereas the adsorption process frequently exhibits nonlinear characteristics. This makes it challenging for PID control to guarantee an accurate control effect in complex systems.In the face of these challenges, the advancement of machine learning has offered a novel strategy for the rapid monitoring and control of adsorption processes, namely model predictive control (MPC). As a significant branch of modern control theory, MPC employs dynamic models to forecast the system's future behavior and subsequently formulates optimal control decisions based on these predictions. Unlike traditional PID control, MPC is capable of handling multi-variable, nonlinear, and constrained conditions, rendering it highly suitable for dealing with the rapid changes and complexities of adsorption processes. This is because there are often multiple interrelated control variables in the adsorption process. By constructing a multi-variable model, MPC can simultaneously take into account the interactions between variables, optimize the global control strategy, and enhance the system's coordination and overall performance.

In addition, MPC can integrate optimal control and constraint processing, which can optimize process metrics such as energy consumption, yield and product quality while meeting various physical and safety constraints of the adsorption process. This constrained optimization ability provides a strong guarantee for the economy and safety of the adsorption process. As depicted in Figure 12a, Moshe *et al.* investigated the application of spectral induced polarization technology for real-time monitoring of the adsorption of organic pollutants within activated carbon filters. By means of laboratory configuration, breakthrough experiments, and reaction-transport modeling, this study established a correlation between

the signal variations detected by SIP and the dynamic progression of solute adsorption in the filter [33]. This approach facilitates the autonomous discrimination and stable operation of the adsorption process. Nevertheless, the challenge of more closely integrating machine learning with real-time monitoring systems has emerged for the application of machine learning in practical working scenarios. As depicted in Figure 12b, Shijie *et al.* designed a real-time monitoring system for the intelligent connected worker manufacturing processes in small and medium-sized manufacturers. This system integrates the state-of-the-art machine learning technology with workplace scenarios for application in advanced manufacturing systems. Specifically, object detection and text recognition models were investigated and employed to enhance the labor-intensive machine status monitoring process, and artificial neural networks were introduced to realize real-time energy decomposition, thus further optimizing the system [34].

In addition to real-time monitoring approaches, there are also studies that integrate visual processes with machine learning models. As depicted in Figure 12c, Rama El-khawaldeh *et al.* put forward a comprehensive computer vision and machine learning model for the automatic real-time monitoring and control of diverse workflows. This research offers methods for rapid data collection and more profound analysis from multiple visual cues through the monitoring of multiple physical outputs. The computer vision model of this study can accomplish real-time visual inspection of the process [34]. Additionally, there exist studies that attain real-time control of the process by employing economy as an indicator. As depicted in Figure 12d, Yeong *et al.* put forward an automated real-time quality monitoring and control system founded on the cost - effective support vector machine. This system explicitly takes into account the cost and error types of inspection. In comparison with the traditional SVM algorithm, CESVM can more effectively incorporate cost factors into the quality monitoring system. This research verified the efficacy of CESVM in enhancing the accuracy of classifying non-conforming products [35].

The application of machine learning in the study of adsorption processes demonstrates great potential. It provides a new approach to solving problems such as the nonlinear modeling of multi-component adsorption, the prediction of key parameters, and the monitoring and control of complex processes that traditional methods struggle with. In the optimization of multi-component adsorption, machine learning breaks through the limitations of traditional models based on simplified assumptions, and can effectively handle the complex interactions and competitive adsorption phenomena among components, opening up new avenues for understanding and optimizing the adsorption behavior of actual complex systems. In parameter prediction, its strong nonlinear fitting ability makes it possible to quickly and accurately predict adsorption isotherms, adsorption amounts, and even difficult-to-measure adsorption energies and other key parameters, significantly enhancing the depth of understanding of the essence of the adsorption process. In the field of process monitoring and control, by combining model predictive control, spectroscopy technology, and computer vision, machine learning enables real-time monitoring and intelligent regulation of the adsorption process, overcoming the shortcomings of traditional PID control in handling nonlinear and multi-variable systems, while also taking into account the economy and safety of the process. However, current applications still face challenges such as large data requirements, insufficient model interpretability, and how to ensure the robustness and reliability of the model in actual industrial environments. Future research should focus on developing more efficient small-sample learning algorithms to alleviate data bottlenecks, improving the physical interpretability of the model to enhance scientific insight, and strengthening the deep integration of machine learning with real-time

monitoring systems. In model design, process risks and costs should be fully considered to promote the development of the adsorption process in a safer direction.

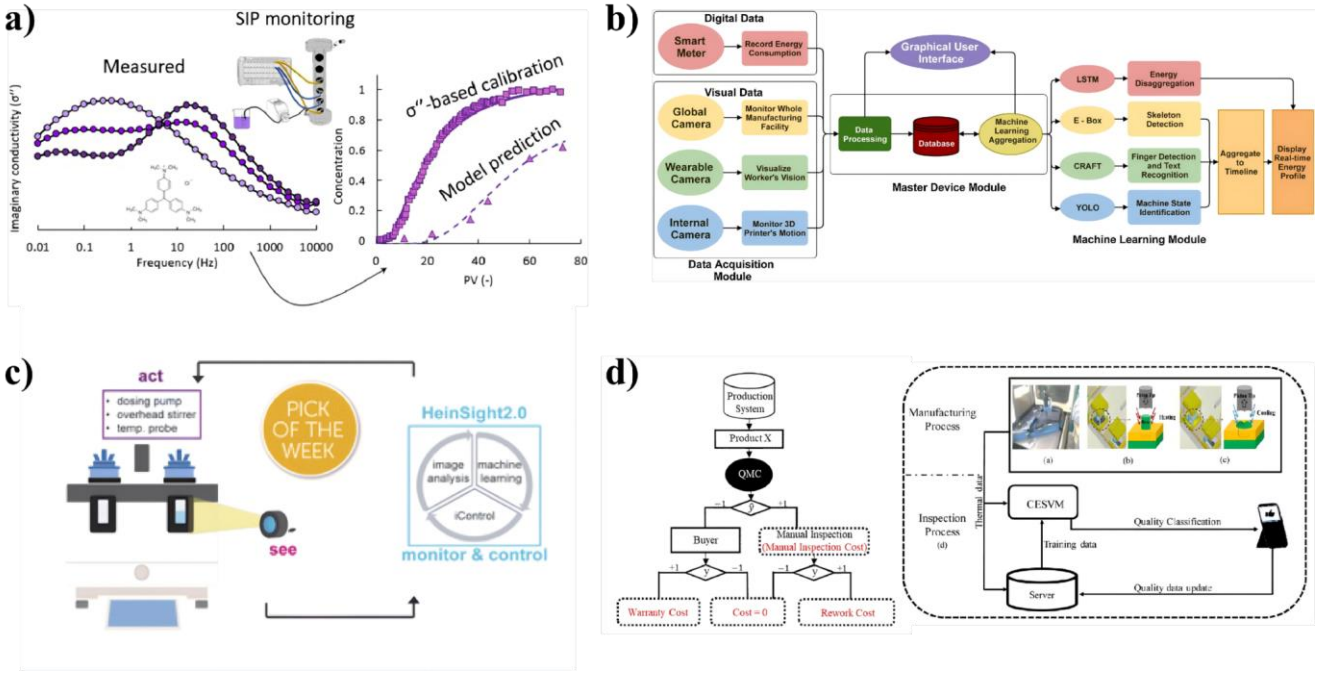

Figure 12. Research on the application of machine learning in the detection of adsorption processes: **(a)** Spectroscopic induced polarization (SIP) was used to monitor the adsorption of organic pollutants by activating carbon filters in real time [33]. Reprinted with permission. Copyright 2021 Elsevier; **(b)** Object detection and text recognition models to improve labor-intensive machine condition monitoring processes [34]. Reprinted with permission. Copyright 2024 The Royal Society of Chemistry; **(c)** Metler-Toledo's iControl software [118]. Reprinted with permission. Copyright 2023 Springer Nature; **(d)** Automated real-time Quality Monitoring System (QMCS) based on Cost-effective Support Vector Machine (CESVM) [35]. Reprinted with permission. Copyright 2024 Springer Nature.

4.3. Machine learning aids reactor design and optimization

The performance of the reactor directly influences the efficiency and product quality of the entire chemical process. The traditional reactor design typically relies on the fundamental principles of fluid mechanics, mathematical models, and fluid dynamics simulations. The expected target is achieved by adjusting the internal structure of the reactor, such as the shape of the agitator, the type of packing, and the channel design.

However, although the design method based on fluid mechanics has effectively controlled the convection behavior, the design of a new reactor not only demands a significant amount of time and resources but also the complexity and variability of experimental conditions often result in model uncertainty and deviation. Moreover, this design method usually depends on experience and heuristic manual adjustment, lacking systematic and automated design optimization, which makes it difficult to rapidly respond to the requirements of new processes and new materials.

In the face of these challenges, the rapid advancement of machine learning technology offers a novel perspective and approach for reactor design. With its powerful data processing and analysis capabilities,

machine learning can effectively extract valuable patterns from extensive experimental data and simulation results, thereby guiding the optimization and innovation of reactor design. By integrating computational fluid mechanics simulations, the machine learning model can quickly evaluate and optimize the flow and reaction distribution within the reactor, enhancing design efficiency and precision.

4.3.1. Prediction and optimization of reactor performance

The present reactor design approach resembles the adsorbent design process in that both employ machine learning to analyze the nonlinear process of the reactor and subsequently optimize the reactor structure. Currently, digital twin technology is primarily utilized in the design of nuclear reactors. As depicted in Figure 13a, Zhao *et al.* developed a simplified thermal-hydraulic model for the nuclear reactor loop system. This study formulated a calculation model for the full-order loop system and validated it. Subsequently, it computed the thermal characteristics of the loop system under different states in the form of snapshots. This research has paved the way for new directions and prospects in the digital twin modeling of the loop system of nuclear reactor systems [36]. The digital twin technology facilitates not only the optimization of the reactor's circuits but also that of the reactor's melting pathways.

In recent years, with the rapid advancement of computer computing capabilities, computational fluid dynamics (CFD) has gradually emerged as one of the crucial technologies for reactor design and process improvement. Likewise, the integration of CFD and machine learning has also become the prevailing research trend at present. As depicted in Figure 13b, Park *et al.* put forward a CFD-based chemical reactor optimization design tool. This tool employs Multi-objective Bayesian optimization to decrease the number of necessary CFD simulations. The developed optimizer can minimize energy consumption and maximize the residence time of gas in an aerated stirred tank reactor [37]. In addition to leveraging machine learning to streamline the computational process of CFD, machine learning can also employ CFD as a data source. By obtaining a substantial amount of simulation data through CFD, the experimental requirements for machine learning can be significantly diminished. As depicted in Figure 13c, Mostafa *et al.* conducted an investigation into the application of porous shell-and-tube catalytic reactors in ammonia decomposition for hydrogen production. This research integrated CFD, ANN, and Response Surface Methodology (RSM) to explore the inherent relationship between the reactor's structure and operation and the system's performance. The study determined that the inlet velocity, inlet temperature, inlet pressure, and porosity were the primary parameters influencing the ammonia conversion rate, system efficiency, hydrogen flow rate, and pressure drop [38].

In addition to acting as a data source for machine learning, machine learning can substantially decrease the computational time of CFD. As depicted in Figure 13d, Zhao *et al.* developed a model with a lower computational cost by integrating CFD and machine learning, with the objective of precisely predicting the carbon dioxide adsorption process. This research indicates that coupling machine learning with the CFD process can not only enhance the interpretability of machine learning but also reduce the computational time of CFD [39].

Integrating the CFD process with the machine learning process represents one of the future trends in intelligent chemical engineering. Nevertheless, owing to the specific discrepancies between the actual reactor preparation in real-world scenarios and the CFD simulation results, the key to the future integration of the CFD and machine learning processes lies in how to achieve the rapid preparation of reactors and subsequently validate the outcomes of the machine learning model.

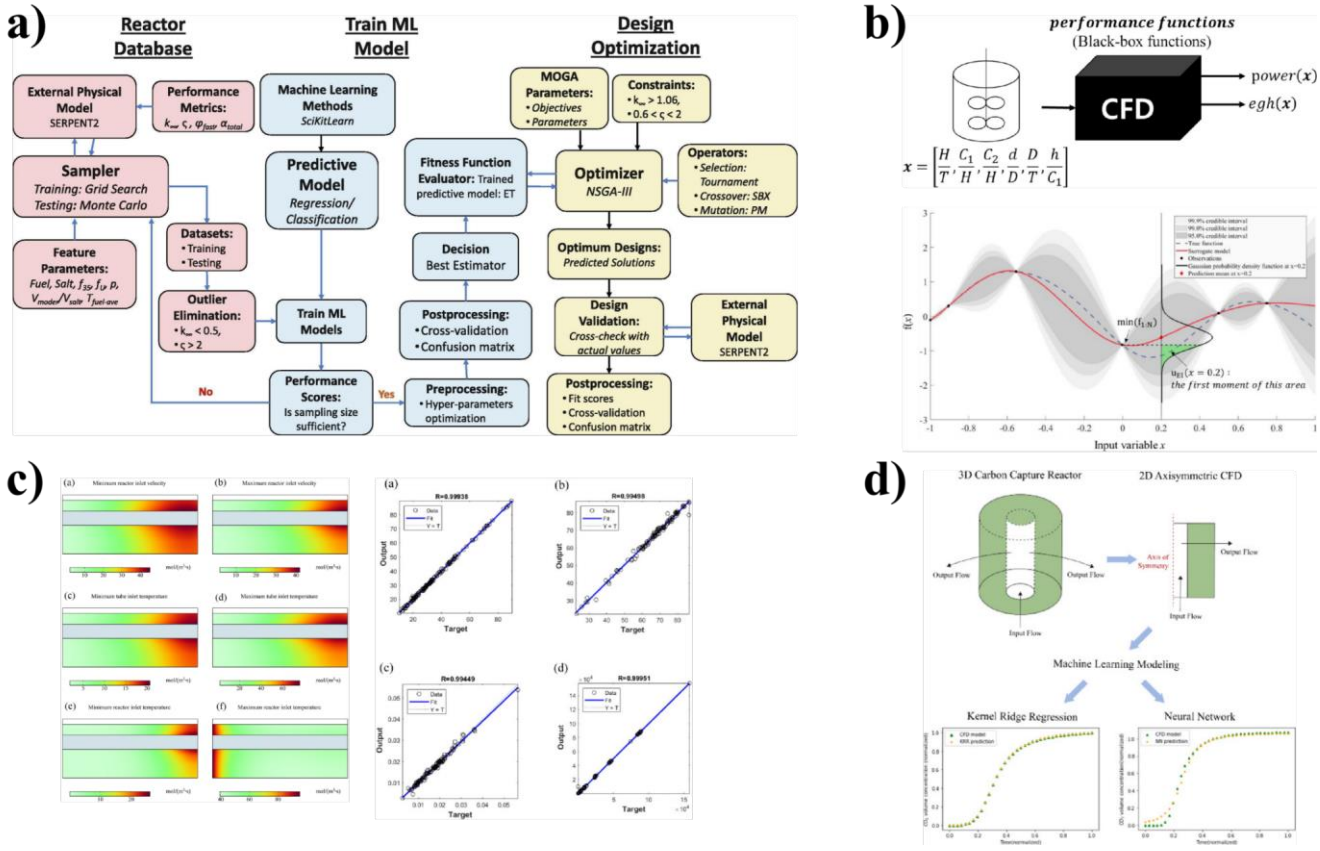

Figure 13. Research on the application of machine learning in reactor design: **(a)** Nuclear reactor design model based on digital twin [36]. Reprinted with permission. Copyright 2021 Elsevier; **(b)** Chemical reaction design tools based on CFD and digital twins [37]. Reprinted with permission. Copyright 2018 Elsevier; **(c)** Response surface method based on CFD, ANN and optimization of reactor process [38]. Reprinted with permission. Copyright 2022 Elsevier; **(d)** Simulation of physical and chemical processes in reactor based on digital twin and CFD [39]. Reprinted with permission. Copyright 2024 ACS.

4.3.2. Reactor simulation based on digital twin

Digital twins are revolutionizing industrial operations in an unprecedented manner. Particularly in the chemical industry, the implementation of digital twins offers a novel perspective and unparalleled advantages for the simulation of adsorption reactors. Digital twin technology, in essence, involves the digital creation of an accurate model in virtual space that corresponds to a physical object or system in the real-world. This model is not merely a static replica but a dynamic digital representation that can be updated in real-time, enabling users to conduct in-depth analyses and optimizations of real-world systems.

In the context of adsorption reactor applications, digital twin technology can precisely simulate the physical and chemical processes within the reactor, thereby assisting engineers and researchers in better comprehending and optimizing the reactor's performance. By leveraging digital twin technology to simulate adsorption reactors, technicians can monitor various parameters within the reactor in real-time, including temperature, pressure, and fluid flow rate. The real-time acquisition and analysis of this data can aid companies in promptly identifying and resolving potential issues, preventing unnecessary downtime and failures, and enhancing productivity. As depicted in Figure 14a, Erbet *et al.* devised a

novel approach for digitizing and modeling the pressure swing adsorption process by leveraging uncertain aware digital twins. The digital twin put forward in this study is characterized by uncertainty awareness and reliability. It undergoes continuous self-updating via online learning and the employment of novel feedback trackers to precisely represent the PSA system. The findings indicate that the proposed method yields a reliable digital twin for the PSA device, which can track the intricate dynamics of the process and adapt to changes, encompassing adsorbent degradation [40].

In addition, digital twin technology also demonstrates unparalleled advantages in the reactor design process. As depicted in Figure 14b, Andre *et al.* put forward a novel software tool concept and its application, which is employed to rapidly and flexibly develop mechanical digital dual-core models of biological processes in various reactor designs. This model encompasses physical-chemical sub-modules and reactor sub-modules. The reactor sub-module is founded on an ideal mixed-stirred tank reactor. The biological dynamics sub-module is decoupled from the reactor sub-module, enabling independent parameterization of the sub-modules. Through the serial connection of these modules, the implementation of the executable digital twin core model wasexpedited [41].

The most significant advantage of digital twin technology resides in its capacity to expedite the rapid design and simulation of reactors under severe conditions. Consequently, the application of digital twin technology to simulate harsh scenarios represents one of the future research directions. As depicted in Figure14c, Gao *et al.* put forward a methodology for constructing a digital twin of the combustion system by utilizing sparse sensing technology. This approach is founded on a model established upon fundamental physical principles. Initially, the model employed CFD to simulate the multi-stage oxygen-enriched combustion chamber of ammonia fuel. Subsequently, an equivalent network of the chemical reactor was established. Thereafter, this research successfully reconstructed the CFD space of selected variables through the application of linear sparse sensing technology, thereby establishing a reduced-order model of the system. The findings indicate that the method proposed in this research can accomplish extensive exploration of the design space and real-time prediction under time-varying operating conditions [42]. As depicted in Figure 14d, Wang *et al.* devised a digital twin platform tailored for the prototype of the four-bed dual-evaporator adsorption refrigeration system employed in the experiment. Leveraging its prediction and optimization capabilities, this digital twin platform is capable of simulating and optimizing the application performance of the adsorption chiller under diverse environmental and load conditions in real-time. This research indicates that, in comparison with conventional methods, optimizing the performance of the adsorption refrigeration machine via the digital twin platform can notably curtail the annual power consumption [43].

Machine learning and digital twin technology provide new ideas for reactor design and optimization. This approach breaks through the limitations of traditional methods based on fluid mechanics and CFD simulations, which are time-consuming, costly, and dependent on experience. Moreover, through powerful data processing capabilities and dynamic modeling abilities, it achieves precise prediction of reactor performance, intelligent optimization of structure, and real-time simulation and control under complex conditions. By combining machine learning with CFD, not only can the computational load be significantly reduced and design efficiency be improved, but the physical interpretability of the model can also be enhanced. The digital twin technology, by constructing a virtual model that is in real-time mapping with the physical entity, provides excellent predictive effects for the entire life cycle of the reactor. However, current applications still face key challenges: First, how to accurately match the

machine learning model and CFD simulation results with the actual preparation and operation of the reactor, which requires more efficient experimental verification methods and data feedback mechanisms. Second, the core of the digital twin model lies in ensuring its high consistency with the real conditions, which depends on high-quality real-time data collection, precise physical modeling, and continuous model update and optimization. To address these challenges, the future development direction should focus on developing hybrid intelligent models that integrate physical mechanisms and data-driven approaches to enhance the generalization ability and reliability of the model. Strengthen the deep integration of machine learning, digital twin, and automated experimental platforms, and build a closed-loop system from virtual design to physical verification. Explore multi-scale, multi-physical field coupling digital twin modeling methods to more comprehensively capture the complex phenomena within the reactor.

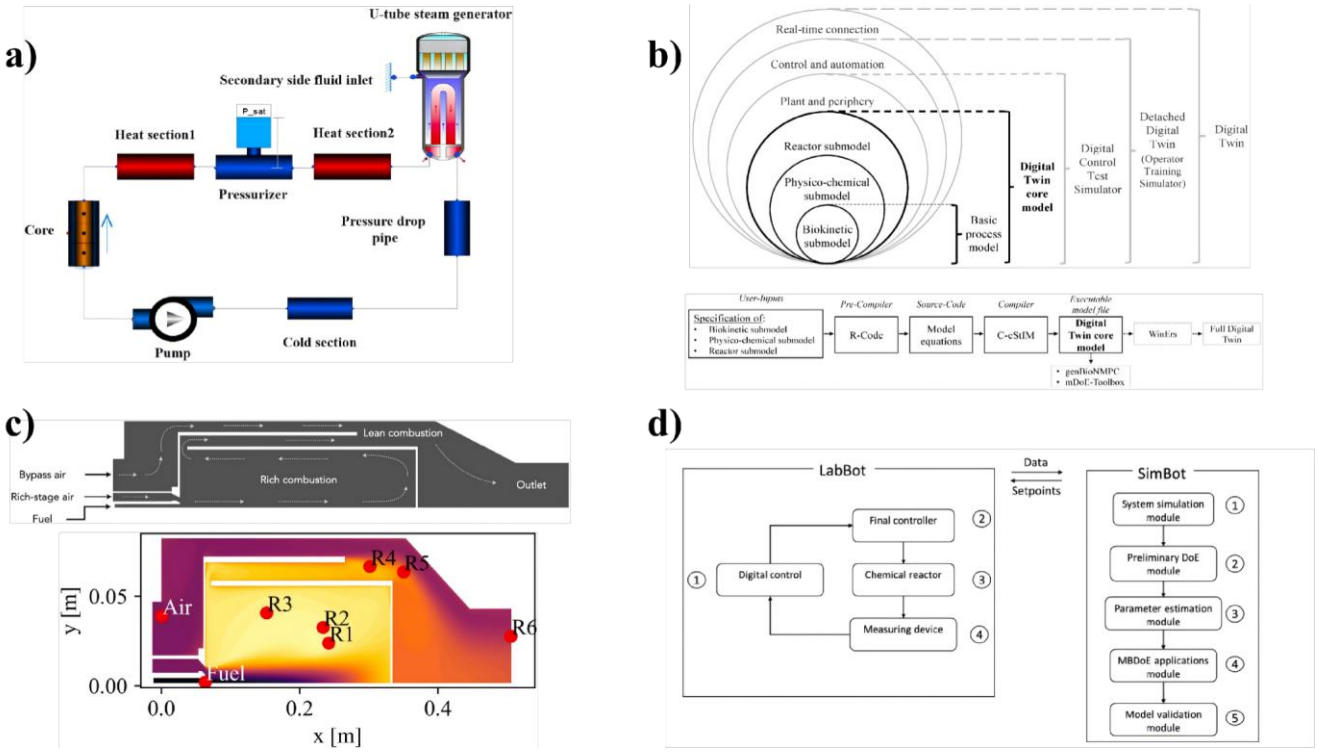

Figure 14. Research on the application of machine learning in digital twins: **(a)** The digital twin pressure swing adsorption (PSA) process of uncertain perception is digitized [40]. Reprinted with permission. Copyright 2024 Elsevier; **(b)** The mechanical digital dual-core model applied to the development of reactors [41]. Reprinted with permission. Copyright 2024 MDPI; **(c)** Digital twin of the combustion system constructed by using sparse sensing technology [42]. Reprinted with permission. Copyright 2024 Elsevier; **(d)** digital twin platform specifically designed for an experimental four-bed two-evaporator adsorption chiller system prototype [43]. Reprinted with permission. Copyright 2024 Elsevier.

4.4. Design of interpretable model aided by adsorption and separation process

In recent years, accompanied by the rapid advancement of machine learning technology across numerous domains, its robust data processing capabilities and predictive prowess offer an entirely novel approach to a multitude of intricate problems. Although machine learning exhibits remarkable potential,

substantial challenges persist in its application. These challenges arise from the fact that the majority of machine learning algorithms are frequently regarded as “black box” models. Their internal mechanisms and decision-making processes are often intricate, and the description of the relationship between data input and output lacks transparency [44,45,119].

The adsorption process encompasses intricate physical and chemical mechanisms, including adsorption equilibrium, adsorption kinetics, surface interactions, and the structural characteristics of porous materials. Among these, there typically exists a high degree of nonlinearity and complexity. This renders it challenging for entirely data-driven machine learning methods to fundamentally uncover the underlying mechanism of the adsorption process, despite their significant advancements in prediction accuracy. This limitation suggests that the “black-box” approach relying solely on machine learning struggles to meet the requirements of adsorption disciplines regarding model interpretability and scientific rigor.

Consequently, to address these issues, integrating artificial intelligence algorithms with the empirical knowledge of traditional adsorption disciplines has emerged as a crucial strategy for enhancing the interpretability of machine learning algorithms. By incorporating domain knowledge into machine learning models, a more profound understanding of the adsorption process can be attained, and the model can become more transparent and scientific.

For instance, Mohd Azfar Shaida *et al.* employed scientific metrology and model-independent multi-layer explainable artificial intelligence (XAI) technology to conduct a comprehensive investigation into the carbon dioxide absorption rate of porous carbon derived from biomass waste. The study revealed that the XGBoost model was the optimal model for predicting carbon dioxide absorption. Subsequently, the best black-box machine learning model served as the foundation for the XGBoost model, and a multi-layer XAI analysis was performed on this model. This model clearly identified the important key features influencing carbon dioxide absorption at the local level [46].

In addition, certain studies have enhanced the interpretability of machine learning models by mitigating their black-box characteristics. As depicted in Figure 15a, Mehdi *et al.* initially constructed a bidirectional interpretable multivariate expert framework for forecasting the monthly SAR values of the river. This framework employs Boruta in conjunction with SHAP incremental feature selection, a set of empirical mode decomposition and variational mode decomposition founded on time-varying filtering, and interpretable Gaussian process regression for interpretation. In this manner, the interpretability and stability of the model can be augmented [120].

There are also studies that acquire the most crucial parameters in the model via traditional approaches. Performing interpretability analysis on these parameters is also a means for machine learning to enhance the interpretability of the model. As depicted in Figure 15b, Zhou *et al.* employed the chemical adsorption energy of reactants on the catalyst surface, and this study regarded Eads as one of the most informative features for comprehending and identifying the optimal catalyst. This study put forward an experimental feature deletion method based on automated machine learning (AutoML), extracting knowledge from a high-throughput density functional theory (DFT) database. The findings indicated that by integrating feature deletion experiments with instance variable selection, an XAI model based on neural networks could be obtained [47].

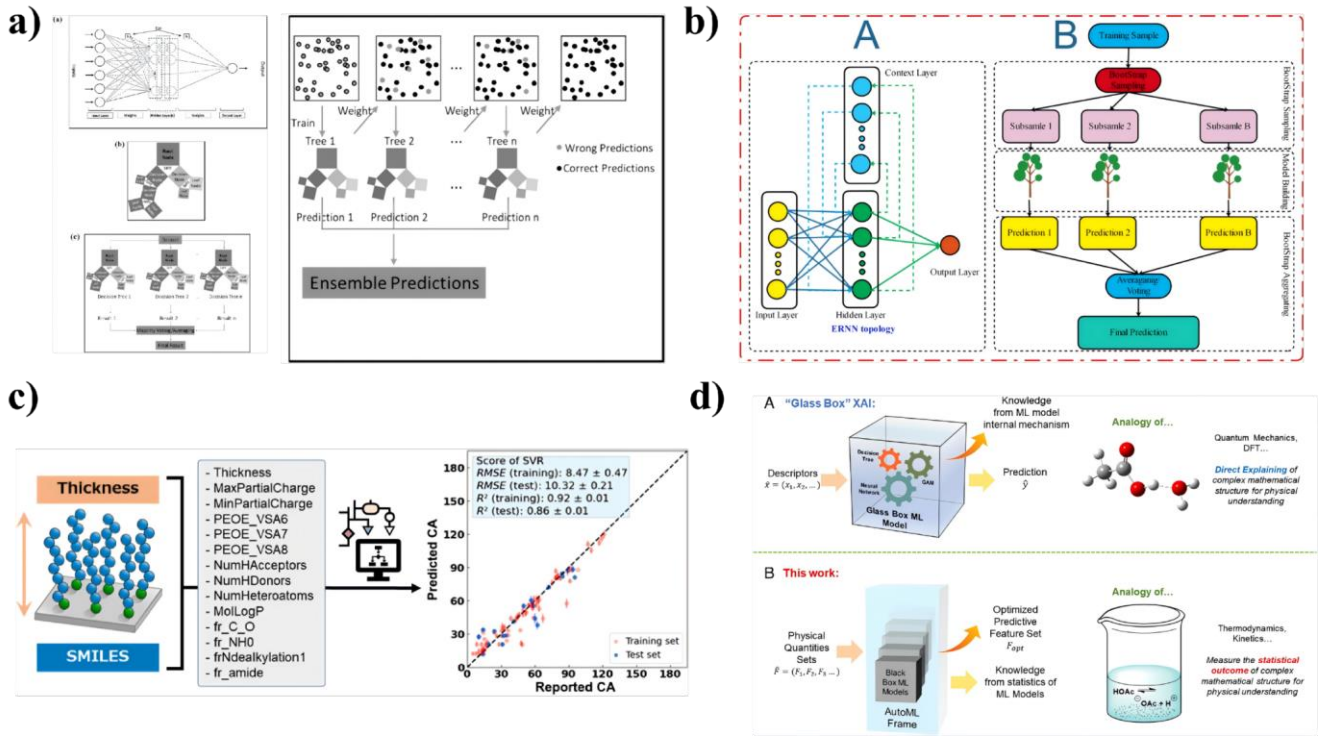

Figure 15. The interpretable machine learning models can be applied in the field of adsorption: **(a)** Bi-interpretable multivariate expert framework to predict monthly SAR on the Zayanderud River in Iran [120]. Reprinted with permission. Copyright 2024 Elsevier; **(b)** Interpretable model using Eads combined with automatic machine learning model [47]. Reprinted with permission. Copyright 2021PANS; **(c)** Shapley additive interpretation combined with BET model to explore explainable model [48]. Reprinted with permission. Copyright 2021 Elsevier; **(d)** Molecular force descriptors combined with machine learning were used to predict the contact angles of polymers [49]. Reprinted with permission. Copyright 2024 ACS.

In addition to chemical stoichiometric strategies such as theoretical calculations, there are studies that leverage the inherent interpretability of machine learning to enhance the interpretability of the adsorption process. As depicted in Figure15c, Kusdhany *et al.* sought to comprehend the hydrogen absorption rate in porous carbon materials. They constructed a machine learning model based on the structure and chemical properties of the carbon material, as well as the excess absorption rate of the material. This research employed Shapley Additive Interpretation to analyze the model. The study revealed that the influence of pore volume on the porous adsorption process is negligible. The pore size distribution is also of great significance, as the correlation between ultra-small pores and excessive adsorption is stronger than that between micropores [48]. In addition to exploiting the interpretability of machine learning itself to deepen the comprehension of the adsorption process, there are also studies that enhance the model's interpretability by selecting suitable descriptors. As depicted in Figure 15d, Su *et al.* put forward a method for constructing a machine learning model based on polymer brushes to establish a dataset. This model is capable of predicting hydrophilicity based on the static water contact angle. This research employs grafting structures and molecular descriptors derived from chemical structures as the characteristic parameters of the polymers. The study demonstrates that appropriate molecular descriptors can enable accurate prediction and understanding of crucial parameters [49].

The black-box nature of machine learning leads to the lack of interpretability of the models, making it difficult to reveal the physical and chemical mechanisms underlying the adsorption process. This is in contradiction to the goal of scientific research to pursue transparency and causal understanding, and has become the main bottleneck for its in-depth application in this field. To solve this problem, current research mainly focuses on integrating the empirical knowledge in the adsorption field with machine learning algorithms, or using explainable AI techniques to extract key features and decision logic from the models, or combining traditional methods such as DFT calculations to obtain parameters with clear physical significance as model inputs, thereby enhancing the interpretability and scientific rigor of the models. The future development direction should focus on how to directly obtain physical and chemical parameters that can explain experimental phenomena through machine learning models. This requires further development of hybrid intelligent models that integrate physical mechanisms with data-driven approaches, coupling first-principles calculations, molecular simulations, and other theoretical methods with machine learning, while designing more physically meaningful feature engineering strategies and iteratively optimizing the models through active learning and experimental verification, so that machine learning can not only accurately predict but also become a powerful tool for revealing the intrinsic laws of adsorption processes and guiding the design of new adsorption materials.

4.5. Research on the synthesis of MOF materials using machine learning

Metal-Organic Frameworks (MOFs) are a class of porous crystalline materials self-assembled from metal ions/metal clusters and organic ligands via coordination bonds. Their unique topological structures endow MOFs with ultra-high porosity and extremely large specific surface area, while simultaneously featuring structural designability and functional tunability [121,122]. These core characteristics enable MOFs to exhibit irreplaceable application potential in the field of adsorption, with wide applicability in scenarios such as gas separation, pollutant removal, energy storage, and catalysis-assisted adsorption, making them a research hotspot in the current fields of materials chemistry and separation engineering [123,124].

However, the synthesis process of MOF materials faces significant complexity and uncertainty. This issue stems from the high diversity of their building units and the strong sensitivity of synthesis conditions, which severely restricts the large-scale preparation and application implementation of MOF materials. From the perspective of building units, the selection of metal ligands covers transition metals, rare-earth metals, and alkaline-earth metals, with significant differences in coordination number, charge distribution, and coordination preference among different metal ions. Organic ligands can be classified into aromatic carboxylic acid types, nitrogen-containing heterocyclic types, and multi-functional group types; the length, rigidity, and functional group type of ligands directly determine the topological structure and pore characteristics of MOFs [124,125]. The combination of these two components can theoretically form millions of potential MOF structures. Nevertheless, in actual synthesis, precise matching of the coordination compatibility between metals and ligands is required; otherwise, amorphous precipitates or impurity phases are prone to form, significantly reducing the yield and purity of the target product. From the perspective of synthesis conditions, the crystallization process of MOFs is extremely sensitive to reaction temperature, solvent type, pH value, reaction time, and post-treatment processes. This sensitivity to the synthesis process makes traditional MOF synthesis rely on empirical guidance, adopting a trial-and-error method plore synthesis parameters. This not only consumes substantial reagents and time but also makes it difficult to achieve directional synthesis of target structures,

resulting in most theoretically designed MOF structures failing to be converted into practically usable materials and forming a dilemma of abundant theoretical structures but scarce practical material.

ML provides a data-driven solution for the synthesis and performance optimization of MOFs. By mining the structure-synthesis-performance correlation laws in MOF databases, it enables rapid screening, directional design, and efficient synthesis of MOF materials. In recent years, ML models based on MOF databases have achieved multi-dimensional optimization: In terms of synthesis parameter optimization, Farhan Zafar *et al.* constructed 8 types of ML models to optimize the metal precursor concentration and sulfur-doped graphitic carbon nitride loading of bimetallic FeCo squarate-based MOF (FeCo-Sq MOF), with the goal of minimizing the overpotential of the Oxygen Evolution Reaction (OER). The research results showed that the decision tree regression model exhibited the best performance among all models due to its advantages of no need for data distribution assumptions, ability to capture non-linear relationships between features, and strong interpretability. It could clearly reveal the influence mechanism of each factor on overpotential, ultimately reducing the OER overpotential of the ML-optimized material to 310 mV [126]. In terms of material performance prediction and screening, He *et al.* proposed an integrated strategy of High-Throughput Computational Screening to screen high-performance materials suitable for NF_3/N_2 separation from the CoRE MOF database containing 10,143 MOFs. The separation performance of 3821 MOFs was calculated via Grand Canonical Monte Carlo (GCMC) simulations, and 6 types of ML models such as CatBoost and XGBoost were constructed to predict TSN values. The results indicated that boosting algorithms significantly outperformed Random Forest (RF) in prediction accuracy due to their ability to effectively capture the non-linear relationships between structural features and separation performance; among them, the CatBoost model showed the best performance due to its efficient processing capability for categorical features, successfully identifying DOYBEA (A520) as the optimal candidate MOF. Experimental validation demonstrated that A520 had an NF_3/N_2 selectivity of 65.16 and a working capacity of 1.70 mmol/g, and breakthrough experiments could achieve the recovery of NF_3 with a purity of 99.99%, confirming the reliability of ML-assisted screening [127]. In terms of performance prediction and synthesis feasibility evaluation of MOFs with complex structures, Kim *et al.* constructed a MOF synthesis feasibility prediction model (PU-CGCNN) using Crystal Graph Convolutional Neural Network (CGCNN) combined with Positive-Unlabeled (PU) learning. Using the CoRE database containing 10,143 experimental MOFs as positive samples and the hMOF database containing 137,953 hypothetical MOFs as unlabeled samples, the model achieved a synthesis feasibility prediction accuracy of 99.87% for experimental MOFs and only 0.01% for hypothetical MOFs, successfully reducing the high-throughput screening range of hydrogen storage MOFs from 100,000-level to 100-level. The vanadium-based MOF synthesized based on the screening results exhibited a total hydrogen storage capacity of 9.0 wt %/50.0 g/L at 77 K and 150 bar, with no performance degradation after 100 cycles, confirming the application value of this model in the directional synthesis of MOFs [128].

Machine learning provides a powerful data-driven solution to address the complexity in the synthesis process of MOF materials. By uncovering the correlation patterns between material structure, synthesis methods, and adsorption performance, it enables rapid screening, targeted design, and efficient synthesis of MOF materials, significantly enhancing the research and development efficiency. However, current applications still face several challenges: Firstly, the completeness, standardization, and data quality of MOF databases need to be further improved. The absence of experimental condition records and differences in characterization data affect the training effect and generalization ability of the model.

Secondly, the differences in synthesis equipment and operating conditions among different laboratories make it difficult for the model to be directly applied. Although multimodal data fusion can to some extent alleviate this problem, a more universal solution is still needed. Thirdly, the black-box nature of some machine learning models limits the revelation of the intrinsic mechanism of MOF synthesis and fails to meet the demand for interpretability in scientific research. Fourthly, the conversion efficiency from machine learning virtual screening to actual synthesis still needs to be improved. Many theoretically excellent MOF structures are difficult to be stably prepared in the laboratory. To address these challenges, the future development direction should focus on: constructing a more complete and standardized MOF database, integrating experimental, computational, and characterization data to ensure data quality; developing hybrid intelligent models that integrate multimodal data and physical mechanisms to enhance the generalization ability and interpretability of the model.

4.6. Research on ransformer-based adsorption energy models

Machine learning driven evolution and application value of adsorption energy prediction as a core quantitative parameter characterizing the thermodynamic equilibrium and kinetic behavior of adsorption systems, the accurate determination and estimation of adsorption energy are of crucial significance for revealing adsorption mechanisms, screening high-efficiency adsorbent materials, and optimizing adsorption process parameters. In the theoretical research and engineering applications of adsorption processes, adsorption energy directly determines the magnitude of adsorption equilibrium constants, the saturated capacity of adsorbents, and the adsorption kinetic rate of target substances: low adsorption energy typically corresponds to weak interactions such as physical adsorption, making it suitable for dynamic separation scenarios where adsorbates require rapid desorption; high adsorption energy, mostly derived from chemical adsorption or strong electrostatic interactions, is more applicable to the deep removal of target pollutants or the immobilization of specific substances [129,130]. Traditional approaches for obtaining adsorption energy mainly rely on experimental measurements and quantum chemical calculations, both of which have significant limitations in efficiency, scale, and applicability, making them difficult to meet the current demands for high-throughput development of adsorbents and research on complex adsorption systems. From the perspective of experimental measurements, adsorption energy must be indirectly derived through methods such as microcalorimetry, adsorption isotherm model fitting or temperature-programmed desorption. This not only imposes strict requirements on the precision of experimental equipment but also necessitates strict control of operating conditions such as temperature and pressure during experiments.

Additionally, the sample preparation process is complex, and the duration of a single test is lengthy, making it particularly challenging to support large-scale material screening or multi-variable process optimization studies. From the perspective of quantum chemical calculations, although DFT can simulate the adsorbate-adsorbent interaction process at the atomic scale and directly calculate adsorption energy, its computational complexity increases exponentially with the number of atoms in the system [131,132]. For porous adsorbents with complex topological structures or multi-component competitive adsorption systems, a single DFT calculation often consumes computational resources ranging from several hours to several days. Moreover, it is difficult to cover crystal defects during material synthesis and massive potential configurations during adsorption, which greatly limits its application in high-throughput material screening and dynamic adsorption process simulation.

The rapid development of ML technology has provided a key technical pathway for breaking through the traditional bottlenecks in adsorption energy research. Data-driven ML models can mine potential correlation patterns from massive adsorption-related data, construct end-to-end prediction models between input features and adsorption energy, and realize rapid calculation and accurate estimation of adsorption energy, significantly improving research efficiency and scale. For instance, the research team led by Janghoon Ock based their work on the OC20 dataset, which contains a large amount of DFT relaxation data of adsorbate-catalyst systems. They adopted a pre-trained RoBERTa Transformer encoder as the core architecture, completed pre-training on large-scale natural language corpora using a dynamic masking strategy, and subsequently constructed text strings with multiple feature combinations and natural language descriptions to systematically evaluate the impact of different input features on the prediction accuracy of adsorption energy. The results showed that the proposed CatBERTa model could process text inputs through the pre-trained Transformer encoder, effectively capture the key features of the adsorbate-catalyst system, and achieve accurate prediction of adsorption energy without relying on the atomic spatial coordinates required by traditional methods [133]. Furthermore, to address the limitations of single-modal models, Transformer-based language models can be combined with GNNs. Through multi-modal learning strategies, the latent spaces of graph embeddings (structural information from GNNs) and text embeddings (semantic information from language models) are aligned, significantly enhancing the ability of language models to distinguish energy differences among adsorption configurations. Meanwhile, leveraging the autoregressive generation capability of generative large language models (LLMs), text inputs can be generated based on the basic properties of the adsorption systemin the absence of precise atomic structure data, thereby realizing coordinate-independent adsorption energy prediction. For example, the team led by Janghoon Ock constructed a two-stage model framework of "graph-assisted pre-training and energy prediction fine-tuning", integrating Transformer language models with GNNs (EquiformerV2) and using the OC20 dataset as the training basis. This effectively solved the core issues of "structure dependence" and "insufficient accuracy" in catalytic adsorption energy prediction, providing a new paradigm for energy prediction of complex adsorption systems [134].

The adsorption energy model based on Transformer provides a new approach to addressing the efficiency issues in traditional experiments and quantum chemical calculations. This method can directly process text inputs and has the unique advantage of not relying on atomic spatial coordinates, effectively connecting experimental data with theoretical calculations, and opening up new methods for the rapid prediction of adsorption energy. However, current applications still face some challenges, mainly due to the lack of interpretability of high-quality models and the black box nature of complex models, which makes it difficult to reveal the physical and chemical mechanisms behind the adsorption energy prediction. Additionally, existing models mostly focus on static adsorption energy prediction and struggle to simulate the energy changes and evolution patterns during dynamic adsorption processes. Therefore, the future development direction should focus on developing advanced machine learning strategies such as transfer learning, semi-supervised learning, and multimodal fusion to reduce reliance on large-scale labeled data and integrate multi-source information such as text, structure, and spectroscopy, thereby enhancing the model's ability to represent complex adsorption systems. It is also possible to deeply integrate physical and chemical principles with the Transformer model to construct a hybrid intelligent model that combines high-precision prediction capabilities with physical interpretability.

4.7. Research on the Integration of explainable machine learning models with adsorption processes

In machine learning research on adsorption processes, the black box of models remains one of the core bottlenecks restricting their industrial application. Although traditional machine learning models can rely on massive data to explore nonlinear correlations among multiple factors in adsorption systems and achieve high-precision prediction of key parameters such as adsorption capacity, adsorption kinetic rate, and selectivity coefficient, their highly abstract internal decision-making process makes it impossible for machine learning to intuitively explain the causal relationship between specific input features and prediction results. Additionally, it is difficult to quantify the relative contribution of each factor to the adsorption mechanism, resulting in the model's prediction results lacking support from physical and chemical theories. This makes it challenging for engineers to formulate targeted adsorbent design or process optimization plans based on such results [135,136].

To address this issue, research focus has gradually shifted toward the application of interpretable machine learning in adsorption processes in recent years. Through strategies such as model structure optimization, feature attribution analysis, and integration with physical mechanisms, the goal of achieving both high-precision prediction and high interpretability of adsorption processes has been pursued. For example, Jingrui Wang *et al.* focused on the study of heavy metal adsorption by MOFs, combining Shapley Additive exPlanations (SHAP) with partial dependence plots. They analyzed the adsorption mechanism through feature contribution quantification and parameter interaction visualization. The results showed that SHAP could accurately quantify the global contribution of five types of features in the field of MOF adsorption, among which adsorption conditions and MOF synthesis parameters were the core driving factors, providing clear parameter guidance for the targeted synthesis of MOFs [137]. Wang *et al.* targeting the prediction of organic pollutant adsorption in soil, used the optimally performing extreme gradient boosting model as the carrier and combined it with the Shapley additive explanation tool to analyze the mechanism from two dimensions: global feature importance and local sample contribution. They identified the electronic effect of organic pollutants and soil organic matter content as key influencing factors, while also revealing nonlinear correlations such as the relationship between pH and the ionization state of organic pollutants, and between soil organic matter and the hydrophobicity of organic pollutants [138]. Paramasivan *et al.* adopted a rough set machine learning framework, converting the dataset of dye adsorption by hydrochar into an information table of conditional attributes-decision attributes. After eliminating redundant features through attribute reduction, they generated interpretable IF-THEN decision rules. First, they determined solution pH, adsorption temperature, and the initial concentration ratio of dye to hydrochar as core attributes via rough set analysis, then generated reduct sets and corresponding deterministic/approximate rules for rhodamine B and Congo red respectively, providing guidance for the synthesis and process optimization of hydrochar [139].

Beyond the aforementioned strategies that enhance model interpretability through algorithm improvement itself, some studies have integrated DFT with interpretable machine learning to introduce atomic-level physical mechanisms into model interpretation, further enhancing the depth and credibility of interpretation results. For instance, Zhao *et al.* used graphdiyne as a carrier, introduced heteroatoms by replacing 1–3 C atoms, and loaded single transition metal atoms in the cavities to construct 120 potential catalytic systems. They first obtained structural features, electronic features, and hydrogen adsorption Gibbs free energy through high-throughput DFT calculations, then used random forest as the

prediction model and combined it with SHAP to analyze feature contributions. The results showed that electronic features dominated the adsorption process, with spin magnetic moment and d-band center being the core influencing factors. This interpretation was highly consistent with the physical mechanism of heteroatom doping regulating d-orbital splitting through p-d orbital hybridization in DFT calculations, achieving deep integration of data-driven prediction and atomic-level mechanism analysis [140].

Through strategies such as feature attribution analysis and physical mechanism integration, not only has high-precision prediction of key parameters for adsorption been achieved through machine learning, but also the intrinsic connection between feature contributions and adsorption mechanisms has been revealed, providing new strategies for adsorbent design. However, current applications still face the following problems. Firstly, the physical consistency verification of the interpretation results is insufficient. Most studies only focus on prediction accuracy, ignoring the matching between the interpretation conclusion and the physical and chemical theory of adsorption, even presenting contradictory interpretations that deviate from the basic theory, and lacking further verification through experimental characterization or theoretical calculation, which can easily lead to data-driven deviations. Secondly, the interpretation ability for multi-component adsorption systems is weak. Existing methods are difficult to quantify the dynamic correlations among component concentration ratios, adsorption site competition, and selectivity coefficients in complex systems, limiting the applicability of the model in actual complex conditions. Finally, the engineering operability of the interpretation results is insufficient. It is difficult to convert the mechanism analysis into specific and implementable process optimization schemes, and the model rules are highly dependent on the training data range, which may fail when the actual conditions exceed the data range. To address these challenges, future development directions should focus on establishing a two-way verification mechanism between interpretation results and physical and chemical theories, through DFT calculations, *in-situ* characterization, *etc.*, to verify the rationality of the interpretation conclusions. By developing interpretable models that integrate multiple physical fields and competitive adsorption theories, the analytical ability for complex multi-component adsorption systems can be enhanced.

4.8. The potential applications of AI basic models in the adsorption process

The basic models of artificial intelligence provide core support for research in the field of adsorption through multi-dimensional technical paths. Their applications cover key directions such as general language processing, multimodal fusion, and professional scene adaptation. In the general language models, the fine-tuned LLaMA series derivative models can accurately predict the solute descriptors and improved solvent parameters in the Abraham model, providing reliable data support for the quantification of solvent-solute interaction strength and the selection of solvents for target adsorption systems [141]. Qwen relies on efficient semantic embedding technology to achieve in-depth analysis of text data such as literature and experimental reports in the field of adsorption, thereby facilitating the extraction of key information, the integration of research results, and the construction of knowledge graphs [142]. Although Claude 3 has not been reported in the literature yet, this model possesses the ability to design complex experimental schemes and derive algorithms. In the future, it can be used to construct low-cost technical paths for adsorption-related experiments, significantly shortening the research and development cycle and reducing resource consumption; The T5 model reconfigures core tasks such as adsorbent screening and experimental data processing through the text generation paradigm, efficiently completing tasks such as generating literature summaries, writing experimental

reports, and extracting conclusions, thereby enhancing the standardization and efficiency of text processing [143]. The BLOOM model, leveraging its multilingual adaptation advantages, enables the cross-language integration and sharing of research data in the field of adsorption worldwide, providing support for cross-border academic exchanges and technological [144]. In terms of the application of multimodal models, CLIP achieves the analysis of nitrogen adsorption experimental characterization images, the identification of the appearance features of adsorption materials, and the analysis of the changes in the material's form after adsorption through image-text alignment technology, providing technical support for the visual assessment of adsorption effects [145]. LLaVA, leveraging its ability to fuse visual and linguistic features, has constructed a visual question-answering system for adsorption experiments. It can quickly respond to key issues such as the distribution of adsorption sites and the evolution of surface morphology based on microscopic characterization data like electron microscope images of adsorption materials, thereby assisting in the precise analysis of experimental results [146]. The Gemini model utilizes multi-source data fusion technology to integrate process data such as temperature and pressure during the adsorption process, as well as image data like spectra before and after adsorption. This enables a systematic analysis of the impact of experimental conditions on the adsorption effect, providing a scientific basis for optimizing the experimental process and regulating parameters [147]. In the professional domain models, AlphaFold combines slow feature analysis with metadynamics simulation technology to accelerate the sampling efficiency of key processes such as the opening of protein hidden pockets and the binding of proteins to ligands. It deeply reveals the mechanism of proteins as adsorption carriers, providing theoretical support for the targeted design of protein-based adsorption materials [148]. DeepSeek Coder specializes in the development and debugging of code for numerical simulation of adsorption processes. It can efficiently generate core programs such as molecular dynamics simulation and grand canonical Monte Carlo simulation, significantly reducing the development cost and error rate of simulation calculations [149]. In the specialized research on MOF/COF adsorbents, the targeted application of multiple artificial intelligence basic models has promoted the development of the field towards precision and efficiency: The Uni-MOF model focuses on modeling the correlation between material structure and performance, and through high-throughput calculations and machine learning algorithms, it enables rapid screening of adsorbents and precise prediction of adsorption capacity. Its cross-condition prediction accuracy reaches 0.98, significantly improving the efficiency and reliability of adsorbent screening [150]. The MACE model, with its atomic-level energy and dynamics prediction capabilities, provides high-precision computational support for the analysis of adsorption mechanisms and the quantification of binding strength at adsorption sites. This results in an average absolute error (MAE) reduction of 7.4% to 9.8% in energy prediction, laying the foundation for a deeper exploration of the essence of adsorption processes [151]. The GPT series models adopt the text-driven structure generation as the core technical path, enabling intelligent design and synthesis path planning for MOF/COF adsorbents. The generated instruction-based structural schemes can be directly reused in the experimental stage, accelerating the transformation process from theoretical design to actual preparation of adsorbents. The BERT model conducts quantitative analysis of structure-performance correlations, accurately identifying the key features that affect adsorption performance. It performs exceptionally well in the analysis of adsorption mechanisms and the optimization of adsorbent modification directions. The accuracy rate of key feature identification exceeds 90%, providing clear technical guidance for the improvement of adsorbent performance [152]. The aforementioned basic model is involved in the entire process from molecular parameter prediction,

multi-source data analysis, experimental scheme design to the development of new adsorption materials. It has constructed an intelligent technology system for research in the field of adsorption, effectively promoting the efficient, precise and innovative development of research in this field.

The AI basic model has established an intelligent technical system for predicting molecular parameters, multi-source data analysis, experimental scheme design, and the development of new adsorption materials. This model has promoted the efficient development of adsorption material design. However, current applications still face many challenges. Firstly, the reliability and generalization ability of the model need to be verified, especially in complex and dynamic actual industrial scenarios, the accuracy and applicability of its prediction and design results still require a large amount of experimental verification. Secondly, the quality and standardization level of data in the adsorption field are insufficient, and the integration of multi-source heterogeneous data is difficult, which affects the training effect and cross-platform application ability of the model. Moreover, most AI basic models still have the "black box" characteristic, their decision-making process lacks interpretability, and it is difficult to ensure consistency with physical and chemical principles, limiting their deep integration in scientific research and engineering applications. Finally, the closed-loop combination of AI models and experimental verification is not tight enough. How to quickly convert model predictions into experimental schemes and optimize the model using experimental feedback remains a key problem to be solved. To address these challenges, the future development direction should focus on improving the generalization ability and reliability of the model through strategies such as multi-source data fusion and reinforcement learning, and strengthening validation and application in actual industrial scenarios. By promoting the standardization and sharing of data in the adsorption field, a high-quality dedicated database should be constructed. Develop interpretable AI technology that integrates physical mechanisms to enhance the transparency and scientific rigor of model decisions.

5. Future development direction and prospect analysis

5.1 Optimization AI model for adsorption process

Although the application of artificial intelligence in adsorption separation technology is gradually expanding, the current application level remains relatively elementary. It primarily focuses on leveraging AI to predict and optimize parameters in the separation process, aiming to enhance separation efficiency and reduce operating costs. At this stage, the core function of AI technology is manifested in handling the relationship between data and optimizing process parameters. However, its profound comprehension of the structure of adsorption materials and the separation mechanism remains inadequate. Simultaneously, AI has not achieved qualitative breakthroughs in assisting process optimization, material innovation, and automation of separation processes. Moreover, there is limited research on explainable AI models based on machine learning in industrial applications.

Looking ahead, to achieve energy conservation and carbon reduction in the adsorption separation process and progress towards the "Intelligent 2.0" stage, apart from addressing new material design issues, the following challenges need to be resolved:

(1) AI-assisted cross-scale research on the adsorption mechanism.

(2) AI-assisted chemical adsorption Intelligence 2.0.

(3) AI-assisted scaling-up of chemical equipment.

5.1.1. High quality data acquisition and database establishment

The collection of high-quality data and the establishment of databases are the cornerstones for promoting machine learning to optimize processes and new materials. Although there are already many public databases available for the performance analysis and research of adsorption materials, as shown in Table 3, due to the fact that the adsorption process is essentially a complex process controlled by multiple steps, many external factors of the materials will affect their adsorption performance, such as hydrodynamic factors that affect liquid film mass transfer, and the structure and differences of the reactor, which will greatly affect the performance of adsorption materials. The above-mentioned databases mainly focus on the static characteristics of the materials themselves, but none of them have well covered the hydrodynamics and reactor differences in the adsorption process. Therefore, it is very necessary to establish computational fluid dynamics databases for different reactor types in the future.

Table 3. Summary of common adsorption databases.

Database Name	URL	Data Type	Advantages	Disadvantages
NIST ISODB	https://adsorption.nist.gov/isodb	Experimental adsorption isotherms (over 32,000 data points), multi-component adsorption data, breakthrough curves	The data is highly standardized, providing JSON format and API interfaces, supporting IAST calculation and simple column breakthrough simulation, and the data is highly authoritative.	Lack of information on fluid dynamics and reactor structure, and the naming of some materials being ambiguous, can easily lead to confusion.
MOFX-DB	Metal Organic Framework Database | Mofs	Calculated adsorption data (more than 3 million data points), covering adsorption-related data of 160,000 metal-organic frameworks (MOFs) and 286 zeolite types	It achieves interoperability with the data format of NIST ISODB with strong compatibility, contains complete grand canonical Monte Carlo (GCMC) simulation metadata, and is well-adapted for high-throughput computational analysis of adsorption properties.	The database only includes equilibrium adsorption data and completely lacks mass transfer kinetics and reactor-scale related data, resulting in significant limitations in its practical application scenarios.
CoRE COFs	Welcome to CoRE COF Database! CoRE-COF-Database	Covalent organic framework (COF) crystal structure data coupled with corresponding adsorption performance data	As a high-quality COF-specialized database, it has a high level of data regularization and is suitable for machine learning research and the establishment of structure-property relationships of COFs.	The database has a relatively small data volume, covers a limited range of gas species, and lacks sufficient dimensionality in adsorption data for COFs.
ARC-MOF	https://doi.org/10.5281/zenodo.6908727	Electrostatic potential-fitted atomic charges calculated by DFT, covering more than 280,000 MOF materials	It provides high-precision DFT-level atomic charge data, which is applicable for high-accuracy molecular simulation and in-depth research on adsorption mechanisms of MOFs.	The data generation involves high computational costs, and the database has a low update frequency, making it difficult to timely include newly developed MOF materials.
QMOF	https://gitcode.com/gh_mirrors/qm/QMOF/	Multi-dimensional data of MOFs including crystal structure, DFT-calculated band gap, and adsorption properties	It is interconnected with the Materials Project database, features user-friendly API interfaces, and supports batch data retrieval and cross-database linked analysis of MOF properties.	Account registration is a prerequisite for database access, and partial high-precision data is subject to permission restrictions, which prevents ordinary users from obtaining the complete dataset.
CSD MOF Collection	https://www.ccdc.cam.ac.uk/	MOF crystal structure data (more than 72,000 entries), including structural descriptors such as largest cavity diameter (LCD), pore limiting diameter (PLD), and helium void fraction	The crystal structure data is complete and detailed, and the database achieves high compatibility with porous material analysis software such as Zeo++.	Adsorption performance data is a core deficiency of the database; additional GCMC calculations are required to acquire adsorption-related characteristics of MOFs.
IZA Database	https://www.iza-structure.org/databases/	Core structural data of zeolites including framework types, topological structures, and pore channel systems	It holds extremely high authority in the zeolite research field, comprehensively covers all known zeolite structures, and serves as a core reference database for zeolite-related studies.	The database has a single data type, only focuses on traditional zeolite materials, and does not cover emerging porous materials such as MOFs and COFs.

In addition to machine learning models, various simulation methods are widely used, each with its own unique characteristics and corresponding databases. As shown in Table 4, the GCMC is a stochastic

method based on the grand canonical ensemble of statistical mechanics, suitable for equilibrium adsorption simulations, with low computational cost, but unable to represent dynamic processes. The matching databases include CSD MOF Collection and NIST ISODB. Molecular Dynamics (MD) analyzes the dynamic behavior of materials by tracking the trajectories of atoms/molecules. Although it has high computational cost and limited time scale for large systems, it is suitable for Materials Project and CSD. DFT is a quantum chemistry method with high accuracy at the electronic scale, suitable for calculating properties such as band gaps, but has high computational cost for large systems and is incompatible with Materials Project and QMOF. Regular Monte Carlo (CMC) can perform stable equilibrium simulations of closed molecular systems, but cannot handle open systems. The matching databases include CSD and COD. Ab initio Molecular Dynamics (AIMD) combines DFT with MD and can perform real and complex reaction simulations without the need for empirical force fields, but has extremely high computational cost and is only suitable for Materials Project and ARC-MOF. Combining these models with machine learning models is one of the methods for optimizing and correcting data sources in the future.

With the rapid development of generative artificial intelligence technology, it has shown unprecedented potential in the fields of materials science and chemical engineering, capable of generating a variety of data including the geometric structure, microstructure, and process performance of materials. This approach can significantly reduce experimental costs and time [153,154]. However, generative AI still faces many challenges and risks in practical applications [155]. Recent studies have confirmed that generative AI first has the problem of hallucination, that is, the generated results often produce content that seems reasonable but actually does not conform to physical laws, such as fictional molecular structures that violate chemical bonding principles and incorrect experimental synthesis paths [156]. Secondly, there is insufficient data accuracy. The performance of machine learning models depends on the quality of training data, and noise and bias in the data can greatly reduce the accuracy of the generated data [157]. Finally, there is the problem of overfitting, that is, the model may overlearn specific patterns in the training data, resulting in poor generalization ability on new data [158]. Therefore, generative AI is most suitable for small sample supplementation and exploratory research, to expand the training set or quickly explore the vast material space, but is not suitable for high-precision parameter prediction and critical decision-making processes [159]. To overcome these limitations, combining generative AI with physical mechanism constraints is an effective solution, that is, introducing known physical laws such as the Langmuir model in adsorption and mass transfer laws as traditional models as constraints in the model to ensure that the generated data conforms to basic physical laws [160,161]. In the future, deeply integrating machine learning with physical mechanisms to make it a powerful auxiliary tool for experimental verification and physical simulation is one of the mainstream research directions.

Table 4. Summary of simulation method.

Simulation Method	Core Theoretical Principle	Typical Application Scenarios	Key Advantages	Main Limitations	Matched Representative Databases
Grand Canonical Monte Carlo (GCMC)	A stochastic simulation method based on statistical mechanics, simulating molecular adsorption/desorption, insertion and displacement under fixed chemical potential, temperature and volume (grand canonical ensemble) to obtain equilibrium adsorption properties.	Adsorption isotherm prediction, gas separation/storage performance evaluation, pore-size-dependent adsorption analysis of porous materials (MOFs, COFs, zeolites)	High accuracy for equilibrium adsorption simulation; low computational cost relative to dynamic methods; ideal for high-throughput screening of adsorbent materials; compatible with various force fields.	Only applicable for equilibrium state simulation; cannot characterize mass transfer kinetics, diffusion behavior and dynamic adsorption processes; relies on high-precision force field parameters.	CSD MOF Collection, IZA Zeolite Database, NIST ISODB, MOFX-DB
Molecular Dynamics (MD)	Solves Newtonian equations of motion to track real-time atomic/molecular trajectories, revealing dynamic evolution and thermodynamic properties of materials at atomic/molecular scale.	Molecular diffusion, mass transfer kinetics, thermal conductivity, mechanical property analysis, interface interaction simulation of porous/crystalline materials	Captures dynamic behavioral characteristics of materials; realizes full-cycle dynamic simulation; supports analysis of structure-dynamics-property relationships.	High computational cost for large systems; limited simulation time scale (nanoseconds to microseconds); sensitive to force field rationality and simulation parameter setting.	Materials Project, CSD, ICSD, ARC-MOF
Density Functional Theory (DFT)	A quantum chemical simulation method based on electron density functional, replacing wave function with electron density to calculate electronic structure, energy and related properties of materials.	Atomic charge fitting, band gap calculation, adsorption site/energy prediction, catalytic mechanism analysis, crystal structure optimization	High simulation accuracy at electronic scale; reveals intrinsic electronic properties of materials; suitable for mechanism analysis and high-precision material screening.	Extremely high computational cost for large-scale systems; long calculation period; not applicable for high-throughput simulation of macro porous material libraries.	Materials Project, QMOF, ARC-MOF, CSD
Canonical Monte Carlo (CMC)	Stochastic simulation under fixed particle number, volume and temperature (canonical ensemble), realizing system equilibrium and property calculation via random molecular displacement/rotation.	Molecular packing, phase equilibrium, adsorption configuration analysis, small-scale molecular system simulation	Stable simulation process; low computational difficulty; suitable for equilibrium property calculation of closed molecular systems.	Cannot simulate open systems with mass exchange; narrow application scope; limited to fixed-composition material systems.	CSD, COD, Crystallographic Databases
Ab Initio Molecular Dynamics (AIMD)	Combines DFT quantum calculation with molecular dynamics, calculating interatomic forces via quantum theory to drive trajectory simulation without empirical force fields.	Reaction mechanism simulation, surface adsorption /desorption dynamics, high-temperature/pressure material behavior, bond breaking/formation analysis	Eliminates force field dependence; high simulation authenticity; suitable for complex reaction and interface behavior research.	Ultra-high computational cost; only applicable for small-scale atomic systems (dozens to hundreds of atoms); short effective simulation time.	Materials Project, QMOF, ARC-MOF
Ideal Adsorbed Solution Theory (IAST)	A thermodynamic prediction method based on ideal solution hypothesis, calculating multi-component adsorption equilibrium via single-component adsorption isotherms.	Multi-component gas mixture separation prediction, competitive adsorption analysis, rapid screening of adsorbent selectivity	Extremely low computational cost; rapid prediction without full molecular simulation; suitable for preliminary high-throughput screening of multi-component adsorption systems.	Based on ideal solution hypothesis; large deviation for non-ideal adsorption systems; cannot reflect local interaction and structural effects.	NIST ISODB, MOFX-DB, CSD MOF Collection

5.1.2. The mechanism model is deeply coupled with AI

Enhancing the computational precision and velocity of traditional mechanism models: In the realm of the chemical industry, the profound coupling of mechanism models with AI has brought about a revolutionary transformation in process optimization, reaction dynamics analysis, and new material development. The mechanism model offers a systematic comprehension of chemical reactions and substance transformation by delineating the fundamental principles and laws governing reaction processes. Nevertheless, the traditional mechanism model frequently encounters challenges regarding

modeling accuracy and computational efficiency. With the rapid advancement of AI technology, particularly the progress of deep-learning algorithms, researchers can leverage AI to effectively model intricate nonlinear systems and enhance the predictive capacity of mechanism models. Moreover, AI can also bolster the reliability and applicability of mechanism models through automated data analysis, extracting significant features from a multitude of experimental data, optimizing model parameters, and uncovering unknown variables. The amalgamation of this mechanism model and AI can not only expedite the exploration of reaction mechanisms but also facilitate rapid decision-making in multi-objective optimization and foster the intelligent development of chemical processes.

Improving the explainability of AI models: The profound coupling of AI with the mechanism model is of equal significance in terms of model explainability. While deep-learning models demonstrate superior predictive performance, their "black-box" characteristic often impedes researchers from clearly comprehending the model's decision-making process. This is especially crucial for applications in the chemical industry, where safety and compliance mandate that researchers understand the mechanisms of chemical reactions and the factors influencing them. Therefore, enhancing the interpretability of AI models not only contributes to augmenting the credibility of the models but also offers more targeted recommendations for optimizing chemical processes. By integrating known physical knowledge, researchers can introduce interpretability algorithms to analyze the contribution of each input feature to the predicted outcome, thereby furnishing a scientific foundation for the model. This enhanced interpretability aids researchers in identifying critical factors in complex reaction systems, optimizing reaction conditions, and ultimately attaining safe, economical, and efficient chemical production.

5.2. AI-assisted chemical adsorption Intelligence 2.0

5.2.1. AI-assisted adsorption process optimization

In the realm of the chemical industry, with the continuous advancement of technology, the AI-assisted chemical adsorption intelligent 2.0 era has gradually emerged. This era not only signifies the upgrading of technical approaches but also denotes the intelligent development of numerous aspects, including process flow, process diagnosis, and optimization. AI-assisted process flow simulation assumes a crucial role in the chemical adsorption process. By integrating digital twin and deep learning techniques, researchers can construct and simulate diverse process conditions during the adsorption process within a virtual environment. This simulation can not only precisely forecast the adsorption behavior and kinetic characteristics of substances but also rapidly identify the optimal operating conditions through parameter optimization, thereby reducing the cost and time associated with experiments. Moreover, the incorporation of AI can endow the process with dynamic adaptability to wave interference, offering a novel perspective for the comprehension and control of complex chemical adsorption processes.

5.2.2. AI-assisted diagnosis and maintenance of adsorption chemical process

AI-assisted chemical process diagnosis and maintenance ensure the operational efficiency and safety of equipment. Leveraging real-time data collected by sensors and monitoring devices, AI systems can conduct intelligent monitoring, promptly identify system anomalies, and issue early warnings. This early diagnostic mechanism can not only substantially reduce the equipment failure rate but also prolong the

equipment's service life. Simultaneously, in combination with Internet of Things technology, the system can achieve real-time data transmission and remote monitoring, offering more comprehensive decision-making support for operators. This AI-assisted process diagnosis and maintenance approach not only enhances the system's operational efficiency but also promotes the intelligentization of equipment management, laying a solid foundation for the stability and safety of the chemical adsorption process.

5.3. AI-assisted chemical equipment amplification

The core issue in the scale-up of chemical equipment lies in the non-linearity of the mass and heat transfer processes within the equipment during the scale-up. This non-linear process poses challenges for traditional models to precisely predict, and simulating large-scale reaction equipment via CFD is extremely laborious. Consequently, AI is employed to achieve accurate and rapid fitting of the non-linear process during the scale-up, and an optimization algorithm is integrated to optimize the relevant parameters in the scale-up of chemical equipment. Technology is utilized to rapidly fabricate optimized equipment to verify the accuracy and reliability of the AI algorithm results. The incorporation of AI in the scale-up process can assist researchers in exploring the mechanism of the non-linear process of chemical equipment scale-up parameters.

5.4. AI-assisted 3D printing for adsorbent design and reactor fabrication

AI-assisted 3D printing technology is revolutionizing the methods of adsorbent material design and reactor manufacturing [162]. In the field of customized porous material preparation, machine learning algorithms have been successfully applied to optimize 3D printing process parameters, thereby precisely controlling surface roughness and pore structure. Previous studies have compared the performance of five machine learning models, including ANN, SVM, and RF, in predicting the surface roughness of fused deposition modeling (FDM), and found that SVM demonstrated the best generalization ability. Additionally, another study utilized the XGBoost method to achieve high-precision prediction of the surface roughness of vertically printed parts [163]. These studies all indicate the significant potential of AI-assisted 3D printing in structural design. In the preparation of adsorption reactors, AI-driven channel design and digital twin collaborative optimization have become research hotspots. In our previous research, we proposed a CFD-ANN-GA-3DP intelligent design strategy, which utilized CFD simulation to construct an ANN and genetic algorithm (GA) to optimize 3D printing reactor parameters, successfully applied to the continuous synthesis of adsorbents and maintained good adsorption capacity [164]. Further, another study developed a real-time control system based on Soft Actor-Critic reinforcement learning and digital twin technology, achieving 20-millisecond bidirectional synchronization on the Viper X300s robotic arm additive manufacturing platform, providing a new approach for the adaptive manufacturing of adsorption reactors [165]. Moreover, a study proposed a "Smart Recoating" digital twin framework that combines Bayesian optimization to dynamically control the powder spreading process during printing, effectively alleviating the interlayer inconsistency problem [166].

Although 3D printed structured materials have made significant progress in adsorption and catalysis applications, the main problem at present lies in the functional limitations of the printed materials [167]. This is mainly due to the decrease in specific surface area caused by the addition of binders, insufficient thermal stability, and the contradictory balance between mechanical strength and porosity. In addition,

although *in-situ* monitoring techniques such as computer vision and infrared thermal imaging combined with AI algorithms can achieve a defect recognition accuracy rate of 98.6% and support real-time closed-loop control, there is still a lack of effective means for *in-situ* characterization of the specific surface area and pore size distribution, which are unique to adsorption materials [168].

6. Conclusion

Experiment duration and limited model generalization ability have long been challenges. With the rapid advancement of big data and computing capabilities, machine learning technology has brought about revolutionary transformations to adsorption separation technology. Through the analysis of extensive datasets, machine learning can effectively tackle complex nonlinear problems that are arduous to solve using traditional methods, offering novel perspectives and tools for the modeling, optimization, and application of adsorption processes.

This paper elaborately presents the applications of diverse machine-learning models in the adsorption process. ANN offer a reliable means for predicting adsorption properties and optimizing processes by discerning latent patterns and key influencing factors within experimental and simulated data. SVM exhibit excellent performance in scenarios involving small samples, high-dimensional data, and noisy environments, rendering them suitable for classification and regression tasks in adsorption processes. The application of CNN in the structural characterization of adsorbent materials can autonomously extract image features and facilitate the rapid identification and analysis of material microstructures. Recurrent neural networks (RNN) and Transformer possess advantages in the modeling of dynamic adsorption processes, as they can capture intricate dynamic relationships in time-series data and provide a new approach for the dynamic prediction and optimization of adsorption processes.

Furthermore, the application of machine learning in adsorbent design and screening is also deliberated. Through high-throughput screening strategies, machine learning can promptly predict and assess the properties of adsorbents, thereby expediting the development of new materials. For instance, the integration of DFT and machine learning can enable a profound understanding of the relationship between the structure and performance of adsorbents, providing a theoretical foundation for the optimal design of adsorbents. Simultaneously, machine learning can also assist in reactor design and optimization, guiding the optimization of reactor structure and the improvement of reactor performance by simulating and predicting the fluid flow and reaction processes within the reactor.

Although machine learning presents numerous advantages in adsorption separation research, it also encounters certain challenges. Prominently, the “black-box” characteristic of the model, *i.e.*, the internal mechanisms and decision-making processes of the model are difficult to interpret. This makes it challenging to fully trust the prediction results of the model in practical applications, particularly in the chemical industry, which demands high levels of safety and reliability. To address this issue, this paper emphasizes the significance of integrating machine-learning algorithms with empirical knowledge from traditional adsorption disciplines. By incorporating domain knowledge, the interpretability and accuracy of the model can be enhanced, making it more dependable and trustworthy in practical applications.

Finally, this paper anticipates the future development directions of artificial intelligence in the adsorption field. With the continuous technological progress, the application of artificial intelligence in adsorption separation technology will become more extensive and profound. For example, integrating the adsorption process with 3D printing technology can enable the personalized design and

manufacturing of adsorption materials to meet the requirements of different application scenarios. Additionally, in combination with the Internet of Things and big-data technology, real-time monitoring and intelligent optimization of the adsorption process can be achieved, enhancing the operational efficiency and stability of the adsorption system. In summary, the continuous development of artificial intelligence technology will bring more innovations and breakthroughs to adsorption separation technology and promote its wide-spread application and development in various fields.

Declaration of generative AI and AI-assisted technologies

During the preparation of this manuscript, the authors used generative AI tools (Grammarly, DeepSeek) only to improve language and readability. The authors take full responsibility for the content of the manuscript.

Acknowledgments

This work was supported by the National Key R&D Program of China (No. 2022YFE0208300), the National Natural Science Foundation of China (Nos. 22278426 and 21908082), Science Foundation of China University of Petroleum, Beijing (Nos. 2462022YJRC002, 2462025BJRC002).

Authors' contribution

Jiangtao Yu: investigation, methodology, writing—original draft, writing—review and editing. Minmeng Tang: conceptualization, methodology, writing—review and editing. Pakiza Ajibek: conceptualization, methodology, writing—review & editing. Feng Gao: funding acquisition, methodology, writing—review and editing. Wenshuai Zhu: funding acquisition, methodology, writing—review and editing. All authors have read and agreed to the published version of the manuscript.

Conflicts of interest

The authors declare no conflicts of interest.

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